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# **ICASE**

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## INTRODUCTION

The Institute for Computer Applications in Science and Engineering (ICASE) is operated at the Langley Research Center (LaRC) of NASA by the Universities Space Research Association (USRA) under a contract with the Center. USRA is a nonprofit consortium of major U. S. colleges and universities.

The Institute conducts unclassified basic research in applied mathematics, numerical analysis, fluid mechanics, and computer science in order to extend and improve problem-solving capabilities in science and engineering, particularly in the areas of aeronautics and space research.

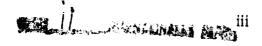
ICASE has a small permanent staff. Research is conducted primarily by visiting scientists from universities and industry who have resident appointments for limited periods of time as well as by visiting and resident consultants. Members of NASA's research staff may also be residents at ICASE for limited periods.

The major categories of the current ICASE research program are:

- Applied and numerical mathematics, including numerical analysis and algorithm development;
- Theoretical and computational research in fluid mechanics in selected areas of interest to LaRC, including acoustics and combustion;
- Experimental research in transition and turbulence and aerodynamics involving LaRC facilities and scientists;
- Computer science.

ICASE reports are considered to be primarily preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period April 1, 1992 through September 30, 1992 is given in the Reports and Abstracts section which follows a brief description of the research in progress.

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#### RESEARCH IN PROGRESS

#### APPLIED AND NUMERICAL MATHEMATICS

#### Saul Abarbanel

Further results have been obtained regarding long time integration of high order compact finite difference schemes approximating hyperbolic systems. A systematic method for constructing the boundary conditions (numerical and physical) was developed. First, a proper summation-by-parts formula is found for the approximate derivative. Next a "simultaneous approximation term" (SAT) is introduced to treat the boundary conditions. An explicit construction of the fourth order compact case is given. Numerical studies verifying the efficacy of this approach were carried out. The above results are presented in an ICASE Report that was coauthored with Mark Carpenter (Fluid Mechanics Division, NASA LaRC) and David Gottlieb.

#### Shapour Azarm

In collaboration with J. Sobieski (Head of IRO) we have developed an approach for reducing the number of variables and constraints, which is combined with System Analysis Equations (SAE), for multiobjective optimization-based design. In order to develop a simplified analysis model, the SAE is computed outside an optimization loop and then approximated for use by an optimizer. The method has been demonstrated by two examples:

(i) a simple explosive actuated cylinder, and (ii) a fairly complex dual-wheel excavator. It has been shown that, for both examples, when the reduction measures are applied they can obtain a solution fairly close to that of the original problem. The small difference in the solution could be eliminated, for example, by increasing the number of variables, constraints, etc., to resolve a lack of sufficient "degrees-of-freedom".

A Paper is being prepared which will soon be submitted to the "Structural Optimization" journal.

#### H. T. Banks

We have continued our efforts in developing an estimation and control methodology for adaptive or smart material structures. Our focus to date has involved piezoceramic devices which are inherently electro-mechanical transducers capable of sensing and actuating. In addition to fundamental modeling (joint efforts with R. Smith and Y. Wang) of piezoceramic

patches as sensors and actuators in beams, plates and cylindrical thin shells, we have developed and used computational algorithms for identification and feedback control. A series of experiments (joint efforts with Y. Wang, D. J. Inman and J. Slater) with piezoceramic actuator/sensor patches bonded to a cantilevered beam have been used to demonstrate the importance of a distributed parameter system approach to address fundamental questions (natural frequencies, mode shapes, damping, etc.) for these structures. We have been able to explain clearly and concisely why the usual engineering modal or finite element (NASTRAN) models for such structures have failed in attempts to produce even the correct natural frequencies. The bonded patches produce local but substantial changes in mass, stiffness and damping that must be accounted for. This can be most readily accomplished with partial differential equations with discontinuous (indeed, unbounded) coefficients and unbounded (involving derivatives of Dirac delta functions) control input coefficients.

These models lead to substantial difficulties in computing feedback control gains. We have, however, succeeded in developing and testing a theoretical (joint with K. Ito) framework for the LQR problem for such models. These ideas are being used in several applications: control of fluid/structure interactions in noise suppression, flow control, and control of high pressure vapor transport reactors for manufacturing of microelectronic devices.

## Kurt Bryan

Work has continued with W.P. Winfree of the Nondestructive Sciences Evaluation Branch, LaRC, on methods for thermal nondestructive evaluation of materials. The recent focus has been on thermal modeling and methods for the testing of interfacial corrosion in composite materials, specifically silicon nitride with embedded silicon carbide fibers. Previous research suggests that the interfacial carbide/nitride thermal properties have a strong effect on the overall thermal behavior of the material and that the status of this interface (a thin carbonrich layer) can be determined effectively by using thermal methods. A mathematical model of the situation has been formulated. A computer program is currently being developed to solve the resulting three-dimensional partial differential equations. In order to obtain reasonably rapid solutions we will use a boundary integral approach and solve the resulting integral equations by using a spectral Galerkin method. The ultimate goal is to derive an algorithm to solve the inverse problem of recovering an estimate of interfacial contact resistance and apply the technique to real data. Also, a real sample of the composite may contain hundreds or thousands of microscopic silicon carbide fibers, and thus the sample may have a quite complicated internal structure. We are thus investigating the techniques of homogenization for partial differential equations, which may considerably simplify the resulting model. However, underlying mathematical model of the composite does not fit the usual assumptions

under which one applies homogenization. Resolving this should give rise to some interesting mathematics.

Work has also continued with Michael Vogelius of Rutgers University and Valdis Liepa of the Radiation Laboratory at the University of Michigan, Ann Arbor. Previously, an algorithm was developed for locating multiple cracks in electrical conductors. The algorithm made use of adaptive applied current patterns in order to provide data which is maximally sensitive to crack locations. Liepa and students built an apparatus to generate data for testing the algorithm and, more generally, exploring the practicality of these techniques and physical principles for nondestructive testing. We used the apparatus to collect data for testing the algorithm and sensitivity of the technique. Some forty different configurations of cracks were tried, with great success. The results will be detailed in a forthcoming ICASE report. We are now looking at applying the techniques of homogenization to the underlying partial differential equation which governs the electrical conduction in order to simplify the model in the case in which many cracks are present.

#### John A. Burns

The development of practical computational methods for optimization based design and control often relies on cascading simulation software into optimization algorithms. The so called "black box" method is an example of this approach. Although the precise form of the overall algorithm may change, there is an (often unstated) assumption that, properly combining the "best" simulation algorithm with the "best" optimization scheme, will produce a good optimal design. There are several examples of real applications where this process fails to produce convergent algorithms, or even worse, produces incorrect converged solutions. There can be several reasons for the failure of the optimal design algorithm (poor sensitivities, non-convergence of adjoint variables, ill-conditioning, etc.), and even if the optimal design algorithm converges to the correct design, then the convergence may be so slow that the method is not useful.

We have worked on several shape optimization and control problems for fluid flow systems. This work has focused on three aspects of computational issues in optimal control and design; (i) fast algorithms for computing sensitivities in Euler flows, (ii) hybrid algorithms for problems with shocks and (iii) fixed finite-dimensional compensators for feedback control of quasi-linear partial differential equations.

We derived a sensitivity equation (SE) method for inviscid, supersonic flows and applied this approach to a problem of shape optimization. The (SE) method is based on solving the linear partial differential equations that are satisfied by the sensitivities. If one uses an iterative (marching) scheme to converge the flow, then the (SE) approach can greatly reduce

the number of flow solves needed to compute sensitivities required by the optimization loop. Perhaps more importantly, the (SE) method can be used to compute a sensitivity with only one mesh generation.

In addition to the work on optimal design, we are continuing our efforts on feedback control of fluid/structure interactions. We have investigated the use of low order compensators to control fluid flows in cases where the number of sensors is small. In particular, we have shown that compensators can be designed for certain non-linear partial differential equations that effectively control the system, even when the full state can not be sensed.

#### David Gottlieb

Research has been proceeding on four fronts including the enhancement of fuel-air mixing by shock-induced vortices, nonlinear Galerkin methods, the effect of inflow boundary conditions on the stability of high order schemes for time dependent methods, and the use of wavelets for solving PDE's.

In the first area, we are addressing computational aspects related to the development of a hydrogen fuel supersonic combustion scramjet that is capable of propelling a vehicle at hypersonic speeds in the atmosphere. In 1990, Marble and his coworkers proposed to enhance fuel-air mixing by optimizing the interaction of fuel and the existing shock wave in a combustion chamber. We are studying the phenomenon by numerically solving the time dependent two dimensional Navier-Stokes equations for the interaction of a shock wave with several numbers of jets. Since detailed features of the flow are required, we use a pseudospectral (Chebyshev-Chebyshev) code which is faster than the ENO code on the Cray. We are in the process of optimizing the shape of the jet (when only one jet is present) and the relative locations of the jets (when more than one jet are present). The spectral code is using theoretical work for the resolution of the Gibbs phenomenon.

We have also been developing nonlinear Galerkin methods (NLG) for the Fourier spectral and pseudo-spectral cases which are relevant to the analysis of homogeneous turbulence in periodic domains. We have started to extend the results of the first stage to include the use of Chebyshev spectral methods in at least one additional direction thus permitting analysis of somewhat more complex geometries. In the process, we have had to clarify the issue of what is meant by "high" and "low" wave numbers in the context of each particular discretization. A first Fourier code for model equations is currently being tested.

On the issue of the effect of inflow boundary conditions on the stability of high order schemes for time dependent methods, it has been recently found that the imposition of inflow boundary conditions may lead to the following problems in the application of high order methods to systems of hyperbolic equations:

- A stable, but nevertheless nonphysical, growth in time is induced in the solution which then falsifies the true features of the solution.
- When one uses time marching techniques, e.g., Runga-Kutta schemes, the intermediate imposition of the inflow boundary conditions leads to the deterioration of the overall accuracy.

These problems are common to all numerical methods: finite differences, finite elements and spectral methods. It should be noted that these problems stem not from the outflow boundary conditions, where numerical boundary conditions are used, but rather from the inflow (physical) boundary conditions.

We have introduced a penalty type (SAT) boundary treatment that overcomes both problems. In the process, a theory has been developed to understand the source of the problems and to prove that the SAT method overcomes it.

The final area of work involves the use of wavelets as basis functions for a collocation technique in solving PDE's. The first task has been to identify the differentiation matrix associated with wavelets. This matrix, which transforms grid point values of a function to the values of the derivative of wavelet interpolants at that set of points, is a product of three matrices. The first matrix transforms the gridpoint values to the wavelets coefficients, the second transforms the wavelets coefficients to the coefficients of the derivative, and the last transforms back to the physical space. In this manner, the wavelet differentiation matrix transforms from physical space to physical space.

In a joint work with L. Jameson, a Brown student, we have constructed these matrices for the Daubechies Wavelets  $D_4$ ,  $D_6$  and higher. The results can be summarized as follows:

- In the case of a uniform grid, the differentiation matrix derived from  $D_4$  is the usual fourth order finite difference scheme.
- In the same case, the  $D_6$  wavelets provide a sixth order finite difference, noncompact formula.
- The wavelets, as with the finite element methods, exhibit superconvergence when boundary conditions are not present. In particular, the  $D_4$  wavelets differentiate exactly forth order polynomials even though they approximate exactly only second order polynomials.
- This provides us with a method of applying wavelets to PDE's in the presence of boundary conditions.

We are currently using the wavelets in their finite difference form to carry out adaptive calculations for systems of hyperbolic equations. We are also checking the question of the superconvergence for different numerical methods. We have shown that superconvergence for the finite elements technique is lost in the present of boundary conditions for hyperbolic equations, and the question under investigation is: Is the superconvergence of the  $D_4$  preserved in presence of boundary conditions?

## Dimitri Mavriplis

Work is continuing on the use of unstructured meshes for solving computational fluid dynamics problems in two and three dimensions.

A new unstructured grid generation strategy has been developed and implemented in two dimensions. The method consists of an advancing front-type algorithm for placing new grid points while employing the Delaunay triangulation criterion for forming new triangles with the new points. The advantages of such an approach are increased efficiency and robustness over other unstructured grid generation methods. This work was presented at the 31st AIAA Aerospace Sciences Meeting at Reno Nevada in January 1993.

A three dimensional unstructured turbulent Navier-Stokes solver has also been developed. This has been achieved by adding viscous terms and a field equation turbulence model to the previously developed unstructured Euler solver. A multigrid method has also been incorporated to accelerate convergence. The code is to be validated on a number of standard 3D test cases in the remainder of the year.

## James Quirk

Having demonstrated that an adaptive mesh refinement algorithm can be used to good effect in the study of reactive shock wave phenomena, work is now in hand to try and unravel the dynamics of the Mach reflection process for detonation waves so as to reconcile the discrepancies between experimental observations and theoretical predictions. Despite the huge computational savings gained via our mesh refinement scheme, the scale of the simulations required for this work is such that we probably need to be able to exploit some form of parallel computing engine to meet our objectives. Therefore work was started with Ulf Hanebutte into investigating ways in which this could be accomplished.

Other work which was started in the last six months includes an investigation into the thermal runaway process associated with the birth of detonation waves (this work is in collaboration with A.K. Kapila, Rensselaer Polytechnic Institute), and a study to determine the extent to which a non-conservative shock capturing scheme can take advantage of our

mesh refinement scheme (this work is in collaboration with S. Karni, the University of Michigan).

## Ralph Smith

In collaboration with H.T. Banks (North Carolina State University), work is continuing on the development of optimal control techniques for the attenuation of noise in acoustic cavities. The model under consideration consists of an elastic structure which is being subjected to a periodic exterior noise source. As energy is transferred to the structure, the resulting vibrations couple with the interior pressure field thus leading to unwanted interior noise. Control is implemented through the excitation of piezoceramic patches which are bonded to the structure. When a voltage is input to the patches, strains are produced which lead to bending moments and/or inplane forces. By incorporating the action of the patches in a fully coupled structural acoustics model for the system, optimal voltages can be calculated via LQR (linear quadratic regulator) optimal control results. As demonstrated by numerical simulations for a 2-D model, the input of these voltages to the patches can lead to substantial reductions in interior noise, and current efforts are being directed toward the application of these techniques to 3-D problems of interest.

Currently, two 3-D models are being studied. The first consists of a thin cylindrical shell with hard endplates. The vibrations of the shell are coupled to the enclosed cylindrical acoustic field through momentum and pressure conditions. Control is implemented through the excitation of curved piezoceramic patches bonded to the surface of the shell. An integral component in the modeling of this system concerns the interactions between the patches and the underlying shell when a voltage is applied. In collaboration with Yun Wang (North Carolina State University), a curved patch/shell model describing these interactions has been developed. The combination of this patch/shell interaction model with shell equations, acoustic equations and coupling conditions yields a fully coupled set of PDE's which describes the response of the system to an exterior noise field and voltage into the patches. The well-posedness of this model has been proven using a semigroup formulation of the problem.

The second 3-D model being studied consists of a hardwalled cavity with a flexible plate at one end. This models an experimental setup being designed and constructed by H.C. Lester and R.J. Silcox (Acoustics Division, LaRC). Control is input through the excitation of piezoceramic patches which are bonded to the plate. Numerical schemes for approximating the dynamics of this fully coupled system have been developed. Through numerical simulations, it has been shown that while the dynamics of the system reflect the individual plate and acoustic components, the plate damping and coupling between the plate and interior acoustic field lead to features in the dynamics that are not easily predicted by considering only

the isolated plate and acoustic responses. This reinforces the need to consider the system as a whole. Current efforts are being directed toward the estimation of physical parameters in the system through data fitting techniques. LQR optimal control techniques will then be used to determine feedback gains for reducing the interior cavity noise.

## Shlomo Ta'asan

The development of efficient multigrid solvers for constraint optimization problems governed by partial differential equations has continued with research proceeding in two directions. The first, which is well developed by now, deals with problems in which the parameter space on which optimization is performed is of finite dimension in the differential formulation of the problem. The methods use relaxation for the parameter space in a multilevel way. Parameters that have a non-smooth effect on the solution are relaxed on fine levels while those of smooth effect are solved for on coarse grids only. The methods use adjoint variables to define a descent direction for the minimization problem. The other direction focuses on problems in which the optimization is over an infinite dimensional parameter space (in the differential level). The same type of ideas for the treatment of the different scales in the problems is being used here. Special attention is given to the numerical processes in the vicinity of the boundary, including new type of analysis to predict the behaviour of different iterative techniques.

The above ideas have been applied in aerodynamics design problems where airfoils are to be calculated so as to meet certain design requirements, for example, to give pressure distribution in some flow conditions which are closest to a given pressure distribution. The present model for the flow is the transonic full potential equation with a body fitted grid. The shape of the airfoil in these calculations is being expressed in terms of a finite number of given shape functions with amplitudes to be found by the design process. Currently, subsonic design problems are being investigated. The goal is to obtain a solution of the optimization problem in a computational cost which is just a few times (2-3) that of the flow solver. At this stage we have been able to show that the design can be done on coarse levels, with essentially optimal convergence rates for fine levels. An effort is being made in reducing the coarse grid work related to the optimization with the hope to get the desired efficiency in total CPU time. This work is jointly done with M. D. Salas (Fluid Dynamics Division, LaRC) and G. Kuruvila (Vigyan, Inc.).

# #

New multigrid solvers for inviscid flow problems are being developed in which the convergence rates are essentially like those of the full potential equation. These methods are based on canonical forms of the inviscid equations in which elliptic and non-elliptic parts of the system are separated. Such representation allow an optimal treatment of the problem.

New discretization methods based on these forms have been developed. These discretizations require numerical viscosity only for the non-elliptic part of the system. The resulting schemes are staggered and admit no spurious (or weakly spurious) solutions even for very small Mach numbers. The schemes are formulated on general grids, structured as well as unstructured, in both two and three dimension. At present we focus on the incompressible and compressible inviscid case working with body fitted grids in two dimension. Flow in nozzle and around a cylinder were considered both for the compressible and incompressible cases.

Another field of study is the efficient treatment of time dependent problems for long integration times. Usually the grids needed for such problems are much finer than those needed for spatial resolution. A method for efficiently calculating the time evolution using mainly coarse grids (depending on the spatial resolution only), has been developed. Coarse grids use extra source terms to correct their evolution process making it arbitrarily close to the fine grid solution. These source terms are shown to satisfy some equations in general, and are being solved for on the coarse grid together with the main solution. The method referred to as Large Discretization Step (LDS) method yields extremely efficient evolution processes. Experiments with hyperbolic equation with periodic boundary conditions have demonstrated typical efficiencies to be expected. Extensions to general boundary conditions and nonlinear case is the next development stage.

## Roger Temam

Multilevel methods are well known in scientific computing and are much studied in relation to multigrid or domain decomposition methods with an emphasis on linear elliptic problems. The utilization of Inertial Manifolds in scientific computing opens the way for the development of a different type of multilevel method more closely related to the physics of the problems, with an emphasis on nonlinear dissipative evolution equations, such as the incompressible Navier-Stokes equations.

The new multilevel methods stemming from the utilization of inertial manifolds which have been introduced so far include the Nonlinear Galerkin Method and the Incremental Unknowns Method; these methods are adapted to the large time integration of evolution equations. At this time, the nonlinear Galerkin method is being implemented for the numerical solution of the Navier-Stokes equations in two and three space dimensions for homogeneous and nonhomogeneous flows, (in collaboration with T. Dubois, A. Debussche, and F. Jauberteau).

Let us describe briefly the main idea. Nonlinear phenomena are characterized by the superposition and the interaction of a large number of modes and, usually, the nonlinear

interaction of the coupled modes obeys complicated laws that are not intuitive. Inertial manifolds have been introduced as a means for describing the interaction of the low and high frequency components of a flow. Indeed, when it exists, an inertial manifold describes the slaving of the high frequencies by the low frequencies. Hence it is one of the motivations of inertial manifolds to produce a tool for studying the long time behavior of nonlinear dissipative systems and uncovering some structure in the real or apparent chaos of nonlinear dynamics.

More generally, inertial manifolds (IM) and approximate inertial manifolds (AIM) yield exact or approximate slaving laws of the small scale component of a flow by its large scale component. Exact and approximate inertial manifolds produce a differentiated treatment of different components of a flow and they are in essence multilevel methods. With that respect, inertial manifolds are directly related to a developing chapter of scientific computing constituted by the multilevel methods, and the nonlinear Galerkin method produces a new insight in multilevel approximation methods for nonlinear dissipative evolution equations through the utilization of inertial manifolds.

Multilevel methods in scientific computing include the multigrid method, the hierarchical basis method, and related methods in domain decomposition. These methods have been primarily studied in the case of linear problems. Their common starting point is the decomposition of the unknown function into arrays of unknowns which, for various reasons, are treated differently. The starting point of multigrid methods is a distinction between the treatment of low and high frequencies; the utilization of hierarchical bases in finite elements pertain to a related idea while, in domain decomposition methods, the aim is to treat differently different parts of the domain either for some reason related to the physics of the problem or in view of a parallel treatment on a parallel computer.

The multilevel methods stemming from the theory of inertial manifolds pertain to a different viewpoint more closely related to the physics of turbulence.

The multilevel methods associated with inertial manifolds include the Nonlinear Galerkin method and the Incremental Unknown method. They are based on a decomposition of the unknown function into its small scale and large scale components. It is interesting to observe that the small scale or high frequency components of a flow account for a large portion of the total number of unknowns while it carries only a small fraction of the total energy or of the magnitude of the unknown function. The multilevel methods that we advocate here address this computing problem in relation with the information on the dynamics deduced from the study of the attractor and its approximation. They produce a gain in computing time of 50% for DNS (direct numerical simulation) and more for LES (large eddy simulations).

#### John Van Rosendale

Work is continuing on the development of highly parallel multigrid algorithms, with emphasis on the development of algorithms which are robust in the sense that their convergence rate does not depend on the problem coefficients. In joint work with Joe Dendy of Los Alamos, we are developing an MSG (multiple semicoarsened grid) algorithm for the Thinking Machines CM-2, which can handle both anisotropic operators and problems having large coefficient jumps. At the moment, the new algorithms speed is faster than a tuned line-relaxation algorithm based on cyclic reduction, although its overall performance is still not quite as good, since line-relaxation algorithms have better sequential performance. We are looking at ways of improving our more parallel algorithm to compensate for this, and expect such multiple coarse grid algorithms to grow in importance as the number of processors in parallel machines grows.

Another area in which we have begun to work is adaptive refinement for CFD problems. Adaptive refinement is quite effective on relatively smooth problems, but can be prohibitively expensive for problems having shocks or other step discontinuities in multiple dimensions. While shock fitting overcomes this problem, it is difficult to do, and generally requires so much apriori knowledge that it is rarely used on complex problems.

The idea we are exploring is to use oriented adaptive refinement, which not only refines the grid in high-gradient regions, but also moves the mesh to approximately fit the discontinuities. This approach has been shown to work on simple approximation problems, and we are in the process of testing it on transonic flow problems in two dimensions.

A related research area, being explored in collaboration with Catherine Mavriplis of George Washington University, is adaptive spectral element methods. Our research here is centered on a new family of triangular spectral elements that we recently developed. Triangular elements provide much greater geometric flexibility than rectangular elements, and are better conditioned and more accurate than quadrilateral elements on domains with sharp corners. However, the lack of efficient tensor product algorithms for triangular elements has inhibited their use. We recently generalized the standard tensor product algorithm for quadralerals to triangles, making it possible to perform efficient spectral element computations on grids containing mixtures of triangular and rectangular elements. The application of these elements and of adaptive spectral methods in several applications areas is currently being explored.

A related idea, which also improves the generality and flexibility of spectral element methods, is the use of Fourier bases. Fourier bases are standard for periodic problems, but spectral convergence can be achieved with Fourier basis on non-periodic problems as well. In particular, we recently demonstrated a Fourier spectral element method which achieves spectral convergence and has better resolution than conventional polynomial element methods. Unfortunately, our Fourier basis is not orthogonal, so some of the attractive properties of the Fourier spectral method are lost. Even so, the improved resolution and improved condition of the new elements suggest they may make an attractive alternative to conventional polynomial element methods.

#### FLUID MECHANICS

## Alvin Bayliss

In work done in collaboration with L. Maestrello (Structural Acoustics Division, LaRC) and J. L. McGreevy (NRC postdoc in acoustics, LaRC), we have begun a study of the role of jet noise in exciting a flexible surface such as an aircraft panel. Specifically we solve the nonlinear Euler equations with a jet flow coupled to an equation governing the response of the flexible surface. The acoustic source is prescribed and we compute the response of the jet and the panel, as well as the resulting radiation from the panel. We consider various aspects of jet noise excitation, including the effect of instability wave and shock generated noise.

In work done in collaboration with L. Maestrello and A. Frendi (AS&M), we consider the problem of computing the radiation from an acoustically excited flexible surface clamped between two rigid surfaces. The problem is solved by coupling the nonlinear Euler equations describing the near and far field radiation to an equation for the evolution of the flexible surface. The pressure difference across the surface acts as a source term.

We consider excitation by an acoustic plane wave at a near resonant frequency and study the behavior as the strength of the acoustic excitation is increased. We consider both the response of the plate and the resulting radiation, which is often nonlinear, into the far field. We have obtained results in both two and three dimensions. An ICASE report describing three dimensional results is in preparation.

## Stanley Berger

We have been continuing our studies of vortex breakdown. In spite of 40 years of research, the basic mechanism causing breakdown is still in dispute. There are various theories based on such concepts as critical states, separation, and stability. Experiments have not been able to resolve the controversy. Numerical simulations have also not provided conclusive results since they have been criticized for various reasons as being unreliable. One of the major criticisms of these latter is that there is a pronounced tendency for the breakdowns to migrate up to the leading computational cell as the numerical integration proceeds. In an attempt to bring some insight into this phenomenon, we have carried out a theoretical analysis which has exposed a very strong elliptic nature to the problem, contributed not by axial derivative terms in the Navier-Stokes equations but instead by the transverse momentum equation which expresses the balance between the radial pressure gradient and the centrifugal acceleration. This analysis suggests that very careful consideration must be given to this ellipticity in carrying out any numerical simulation of breakdown.

We are currently investigating carrying out direct numerical simulations of breakdown, using either spectral methods or compact finite-difference schemes. No studies have yet been reported of vortex breakdown with other than laminar flow, whereas most experiments show clearly the existence of turbulence in the aft portion of the breakdown. Since breakdowns occur at relatively modest Reynolds numbers such direct simulations may represent the real physics of breakdown quite well.

## Fabio Bertolotti

The transition to turbulence in a boundary layer over a flat plate with mild surface undulation has been studied using the xPSE tool-kit. The simulations incorporate the receptivity, the linear growth, and the nonlinear wave interactions leading to "spike stage" and rapid spectrum widening. Both H-type and K-type routes can appear, as well as more complex routes involving the transfer of energy from higher to lower frequency modes. Cases involving waves of sufficiently small amplitude to maintain the flow laminar, could be made transitional by the addition of weak streamwise vorticies. These vortices displayed algebraic growth, whose strength varied with the initial condition selected. A suitable initial condition was developed which produced negligible algebraic growth and is reported in an ICASE report.

The xPSE transition analysis tool-kit has been further optimized, and more powerful post-processing codes have been added. The optimization has lead to a more robust code, capable of better handling the free shear layers under investigation, namely the wake and the Bickley jet.

#### Tom Brown

Laminar flamelet models that describe combustion as stretched 1-D steady laminar flames are promising as sub-grid models of finite-rate chemistry. These laminar flamelet models need to be validated. At Vanderbilt, species concentration and temperature measurements made in turbulent flames using UV Raman Scattering are being compared to 1-D strained laminar flamelet models. Super-flamelet OH values have been discovered in turbulent flames and are being investigated.

In addition, a line Raman system has been developed which is capable of instantaneously measuring species and temperature at multiple points through a flame sheet. This system can provide much needed information about scalar gradients through the reaction zone. The line Raman system is currently being modified to make measurements on 1-D strained flames produced by an opposed jet burner from NASA LaRC. These measurements will be useful

in the validation of flamelet models. The preliminary opposed jet measurements will be compared to computational results at the ICASE summer workshop.

#### John Buckmaster

Certain flames are generated by the combustion of multiphase mixtures - gas and solid particles, or gas and fuel drops. When acoustic waves interact with such flames, instabilities can arise associated with slip (velocity and temperature lags) between the two phases. This mechanism could be responsible for low frequency instabilities observed in gas turbine engines and ramjets. As part of a general study of multiphase flames with acoustic wave interaction, a simple model relevant to the turbine problem has been analyzed. It suggests that the strength of the instability is strongly related to the fuel volatility, in agreement with experimental observations. Work has also been done, with T. Jackson, on the stability of flames containing inert particles in which radiation between the particles is a significant component of the total energy flux. It has been shown that this tends to suppress the cellular instability (Lewis number smaller than 1), but enhances the pulsating instability (Lewis number greater than 1).

## Ayodeji Demuren

Research activity in this period involved the evaluation of Reynolds stress models in turbulent free shear flows, in continuation of previous studies on wall-bounded flows. The goal is to device Reynolds stress closures which can predict accurately the range of simple shear flows comprising of wall boundary layers, jets, wakes and mixing layers. Complex flows are synthesis of these simple flows. Current results show that the SSG (Speziale, Sarkar and Gatski) model which performed very well in plane channel flow may not be sufficiently energetic in mixing layers. Remedies to this problem are now under investigation. Furthermore, its ability to predict secondary motion of Prandtl's second kind in non-circular channels is being investigated. In conjunction with Robert Wilson, the nature of the structures and instability mechanisms in unsteady mixing layers is being investigated. The goal is ultimately to study similar structures in three-dimensional jets.

#### Peter Duck

The work on the interaction between a shock wave attached to a wedge and small amplitude, unsteady, freestream disturbances (with Drs. Lasseigne and Hussaini) is now the subject of a paper currently in preparation. The upstream disturbances may take on the form of acoustic waves, vorticity waves or entropy waves, or a linear combination of all three.

These waves then generate disturbances behind the shock of all three classes. Interestingly, some of these downstream waves, in certain regions of physical and parameter space decay downstream, whilst in other regions, these waves approach a purely oscillatory state. The appropriate regions have been studied in some detail.

The work on the inviscid stability of the "Trailing-line vortex" in the compressible regime has recently been submitted for publication, and has also been published as an ICASE report. This work has been extended to include the effects of viscosity, which has been shown to play a purely stabilising role in the stability analysis. Viscosity has a particularly interesting effect on so-called "center-modes", where the eigensolutions are primarily concentrated at the center of the vortex.

Other work has been involved with the study of flow along a corner, of general angle along with its inviscid stability. The basic flow is determined from the simultaneous computation of three momentum equations together with continuity. There is some disagreeement between the previously published basic flow results, and some of our early computations certainly cast doubt on a number of these previous results.

#### Gordon Erlebacher

Work is still in progress with Shu (Brown University) on the interaction of a shock with an impinging longitudinal vortex. This work has relevance for the stability of aircraft. Some inconsistencies between theoretical and numerical results have been found and are under investigation.

We also initiated research into the physics of shock/turbulence interaction. The final goal of this work is to better understand the behaviour of turbulence as it is processed through a shock. Work has begun with an existing code which is being calibrated for accuracy, and will then be enhanced. Both algorithmic issues and physical mechanisms are being addressed.

Turbulence simulations on the 512 node Touchstone Delta at Caltech are still in progress. We have limited ourselves to 256<sup>3</sup> simulations of compressible turbulence using 1/2 the machine.

We coordinated the organization and execution of ICASE's first shortcourse on the fundamentals of Wavelets from the numerical and applications point of view. With approximately 100 attendees, the course was a big success.

#### James Geer

The problem of determining the acoustic field in an inviscid, isentropic fluid generated by a solid body whose surface executes prescribed vibrations in the presence of a prescribed external flow field is being formulated as a multiple scales perturbation problem. The problem naturally involves two "small" parameters, namely, the Mach number M based on the maximum surface velocity, and the Mach number  $M_{\alpha}$ , based on the external, prescribed flow. Thus, this work extends some previous work on this topic for the same problem with no mean flow present. Following the idea of multiple scales, new "slow" spacial scales are introduced. These scales are defined as the usual physical spacial scale multiplied by powers of M. The governing nonlinear differential equations lead to a sequence of linear problems for the perturbation coefficient functions. It appears that the higher order perturbation functions obtained in this manner will dominate the lower order solutions (as in the case of the zero mean flow case), unless their dependence on the slow spacial scales is chosen in a certain manner. In particular, it appears that the perturbation functions must satisfy an equation similar to a "convective" Burgers' equation, with a slow spacial scale playing the role of the time-like variable. The method has been applied successfully to a simple one-dimensional example, and will eventually be applied to various problems involving a vibrating sphere.

A three-step hybrid analysis technique, which successively uses the regular perturbation expansion method, the Pade' expansion method, and then a type of Galerkin approximation, is also being developed and studied. It is being applied to several model problems which develop boundary layers as a certain parameter becomes large. These problems involve ODE's, PDE's, and integral equations. In particular, the technique appears to simulate these boundary layers by producing approximate solutions with singularities which lie just outside the domain of interest. Based on some preliminary results, the technique appears to provide good approximations to the solution, even when the perturbation and Pade' approximations fail to do so.

Work is also progressing on another new technique, temporarily called the "flexible singularity expansion technique". This technique is being developed to determine a family of approximate solutions, based on a small parameter  $\varepsilon$ , to certain classes of exterior boundary value problems. These solutions are expressed in terms of singular solutions to the governing differential equation for which the singularities lie outside the region of interest. In general, the exact type, location, and strength of these "flexible" singularities are determined by the governing equation and shape of the domain of the problem. More specifically, the various parameters associated with these new singularities are determined by requiring that the "flexible singularity solution" agree with the perturbation solution to the problem to within a prescribed order in  $\varepsilon$  as  $\varepsilon \to 0$ . The technique is being applied to several classes of problems involving nonlinear PDE's and to problems which are geometrically nonlinear.

A new class of approximations S[N, M] to a periodic function f which uses the ideas of Pade', or rational function, approximations based on the Fourier series representation of f,

rather than on the Taylor series representation of f, is being constructed and studied. Each approximation S[N, M] is the quotient of a trigonometric polynomial of degree N divided by a trigonometric polynomial of degree M. The coefficients in these polynomials are determined by requiring that an appropriate number of the Fourier coefficients of S[N, M] agree with those of f. Explicit expressions are being derived for these coefficients in terms of the Fourier coefficients of f. It has already been proven that these "Fourier-Pade" approximations converge point-wise to  $(f(x^+) + f(x^-))/2$  more rapidly (in some cases by a factor of  $1/k^{2M}$ ) than the Fourier series partial sums on which they are based. The approximations are being applied to several model functions, and applications to the solution of a variety of initial, boundary-value problem for several classes of PDE's are being explored.

#### Chet Grosch

During this period I have completed a study of the structure and stability of a three dimensional, compressible reacting mixing layer. The mean flow is formed by two streams at an angle to each other. The effect on the ignition and structure of the flow of of the ratios of free stream speeds temperatures, flow direction and Mach number was calculated. The stability calculations were for three dimensional disturbances in this three dimensional mean flow. In addition, calculations are being carried out in order to model the experiments, done with Michael Gaster, of the boundary layer displacement modes. These calculations involve using boundary layer codes as well as a complete time dependent incompressible Navier-Stokes code. Finally, a study of transition modeling using triple decompositions of the fields has been begun.

## Philip Hall

Work on the receptivity problem for streamwise vortices induced by localized or distributed roughness was carried out. The initial stages of the instability of highly curved flows was investigated, in particular the initial form of vortex-wave interactions in such flows was determined. The instability of the flow in an oscillating rectangular tank was investigated. Results on a generalization of the Kuramoto-Sivashinsky equation were found, these are relevant to the instability of multi-layer fluid flows. Work on the instability of multi-phase boundary layer flows was carried out.

#### Paul Hammerton

Investigation of the propagation of sonic booms through a realistic model atmosphere was initiated. Earlier work by the author, in conjunction with D.G. Crighton at the University

of Cambridge, suggests that for a real atmosphere, relaxation effects associated with internal vibration of polyatomic molecules plays an important role in determining the shock structure. Since relaxation times for air are highly sensitive to the presence of moisture, the relative humidity of the atmosphere may have a significant effect on shock rise-times.

A governing equation was derived taking full account of exponential density stratification, the effect of relaxation processes and the cylindrical spreading associated with a supersonic body. In general the shock rise-time is small compared with the overall pulse duration, and hence an analysis based on the method of matched asymptotic expansions is possible, at least when a single relaxation mode is present. One result obtained is of particular interest. Under certain conditions, the structure of the relaxation shock can change from fully-dispersed to partly-dispersed. Asymptotic analysis of the local change in profile at this point is being pursued.

In addition, a numerical investigation of the same problem was started. For a single relaxation mode dominating the medium, the numerical results will serve to verify the asymptotic predictions, as well as establish their range of validity. The effect of more than one relaxation mode will then be considered. The ultimate aim is the accurate prediction of shock overpressure and shock rise-time on the ground, taking account of the relaxation modes associated with oxygen and nitrogen and the sensitive to atmospheric humidity. Much useful assistance was obtained from other ICASE researchers on suitable numerical schemes and the application of boundary conditions far from the shock front.

## Fang Q. Hu

Research in two areas of aeroacoustics has been initiated. The first area is duct acoustics, associated with the noise reduction schemes for the High Speed Civil Transport(HSCT) project. In particular, the effect of acoustically lined walls on the confined jet noise generation/propagation is being investigated using a linear theory. This work is to provide pertinent information for experimental and computational studies. The second area is in Computational Aeroacoustics in which a spectral method will be used. Aeroacoustic noise spectra often involve sound waves with wavelength/frequency of several orders of magnitudes apart. The challenge is to compute these sound waves with minimum amplification and phase errors. The spectral method provides a very attractive and promising approach for the acoustic problems due to its superior spatial resolution. Work is directed toward using the spectral method effectively.

#### Tom Jackson

Work continues on flame/vortex interactions, a fundamental problem for the understanding of small scale structures in turbulent reacting flows. The role of acoustics on flame/vortex interactions was completed and has just been accepted for publication in the Journal of Fluid Mechanics. Currently, the effect of shear on such interactions is under investigation. A combination of asymptotics and numerics will be used to isolate key physical effects for analysis. This work is in collaboration with M. Macaraeg (Fluid Mechanics Division, LaRC) and M.Y. Hussaini.

In addition, work is continuing on the stability of a three dimensional stagnation point flow. An initial value approach is undertaken to investigate the effect of transients on the evolution of the solution. This work is in collaboration with W. Criminale (University of Washington) and D.G. Lasseigne (Old Dominion University). For reacting flows, disturbances are expressed as an infinite series. When the series is truncated at some large N, a finite number of boundary value systems result for the determination of the growth rate and the flame shape that depends on N, on the cross stream wavenumber and on all the relevant physiochemical parameters. Work has been completed for the planar geometry and is currently being extended to axisymmetric geometry. This work is in collaboration with M. Matalon (Northwestern University).

## D. Glen Lasseigne

The response of the flow field behind a nonreacting shock wave supported by a wedge to general disturbances upstream of the shock has been investigated in detail. Nonlinear aspects of the above interaction using an adaptive numerical code is currently being pursued.

Also under investigation is the non-linear interaction of freestream disturbances and/or wedge movements taking into account the detonation structure of a reactive gas.

The evolution of three dimensional disturbances in a three dimensional stagnation point flow has been studied. Of particular interest is the response of inviscid disturbances within an inviscid mean flow field. The conditions for transient growth in the energy of the disturbances (even though linear theory predicts stability) is explored in detail.

## Geoffrey Lilley

The aim of my work at ICASE was to assist in the development of the newly created field of Computational Aeroacoustics and its major aim in exploiting recent expansions in computer power and the successful growth in the past decade of computational fluid dynamics including the use of DNS (direct numerical simulation) and LES (large eddy simulation).

The expressed hope was that with the integration of the supercomputer into the field of aeroacoustics, complementing current experimental investigations, the methods of prediction of aircraft noise would be enhanced, and our understanding of the mechanisms of noise generation, propagation, and radiation from the exhausts of a turbojet engine would be improved. I collaborated with Dr. Jay Hardin of the Acoustics Division (LaRC), Dr. Tom Gatski and Chris Kennedy of the Fluid Mechanics Division (LaRC), and many members of the ICASE scientific staff, including Dr. Sutanu Sarkar and Dr. Stephen Otto.

A study was made of current empirical methods of jet noise prediction for subsonic exhaust Mach numbers, in both moving and stationary external flows. Such methods depend on a detailed knowledge of the structure of the spatially growing mixing region from the nozzle exit to far downstream. A review was made of current work on the simulation of the turbulent structure of the spatially growing mixing layer as well as that for the temporally growing mixing layer. This included a re-examination of the recent work completed in collaboration with Professor Philip Morris of Penn State (1990) using the wave theory of turbulence, since this theory had the advantage over current turbulent models in that the temporal characteristics of the turbulence in a spatially developing mixing region could be investigated. In aeroacoustics it is a knowledge of the space-time properties of the turbulent flow that is crucial to an understanding of the generation of noise from a turbulent flow. Such properties are only incompletely understood at the present time. As part of this study an approximate theory was developed for estimating the changes in the growth of the mean vorticity thickness of the early mixing region in a jet with jet velocity or Mach number, velocity ratio, and density ratio. This theory was shown to be in fair agreement with experiment and the work of other authors. Dr. Peter Duck assisted me with these calculations.

At the time I joined ICASE, Dr. Sarkar was making an in-depth study of the noise radiated from isotropic turbulence using DNS methodology. It was clear that this was an important test case in the new field of computational aeroacoustics for all other turbulent flows were more complex and their computational aeroacoustics for all other turbulent flows were more complex and their computation depended critically on a successful outcome to the predictions of the noise radiated from isotropic turbulence. An analytical treatment of this problem had been studied by Proudman (1952) and since the early results of Sarkar showed major differences with the work of Proudman, it appeared important that Proudman's work needed to be reappraised, including the assumptions made, the conclusions and the results. This was carried out and it was found that an improvement to that theory could be established in which the assumption of the neglect of retarded time differences could be dispensed with. However the final results were not greatly affected by the addition of this

correction. The differences with the results of Sarkar were resolved to the extent that in the DNS method, greater time resolution was demanded together with considerably longer run times. The results of this work are in the course of preparation for publication.

As discussed above, the prediction of the noise generation from the turbulent mixing region of a jet demands a detailed description of the space-time structure of the turbulent flow. An important length-scale parameter is the rate of growth of the mixing region and its changes with jet Mach number and density ratio. It was decided that prior to an in-depth numerical attack on the mixing region turbulent structure, it was essential to have an improved understanding of the mean flow properties over that currently available, and including the approximate theory developed earlier. Accordingly a self-preserving theory of the compressible turbulent mixing region was developed giving the mean velocity, temperature and density distributions for various Mach numbers, and velocity and density ratios. This work was performed in collaboration with Dr. Stephen Otto, and is in the course of preparation for publication. This phase of the work on the mean flow involving the mean turbulent structure of the mixing region was extended to study the unsteady flow characteristics. This aspect of the work is continuing.

## Stephen Otto

During a visit to the University of New South Wales (UNSW), investigations were continued into the inviscid instability of some nonlinear vortex states. In particular, the three dimensional Rayleigh equation was solved to determine the temporal stability of a state comprised of the most unstable Görtler mode and its harmonics. This mode occupies a thin layer within the conventional boundary layer. This work is joint with J. P. Denier of UNSW and concurrent studies are also being affected which concern a nonlinear Taylor vortex state. It is not clear if the presence of a vortex will increase or decrease the stability of already inflectional state. Work is currently being done with P. Hall (University of Manchester, United Kingdom) to investigate the effect that the presence of vortices has on the stability of some shear layer situations. The calculation is being affected for shear layers in incompressible, compressible and stratified fluids. In the latter of these problems, there is a definite stability bound (dependent on the Richardson number of the flow) for the two-dimensional state and it will be interesting to see if the three-dimensionality will circumvent this.

In a similar vein, work with C. L. Streett (Theoretical Flow Physics Branch, LaRC) has begun, with a view to investigating flows which are generated from numerical simulations. We wish to determine whether the temporal inviscid stability of a state can be used as a breakdown criterion. This is being investigated for two physical situations: rotating disk flows and swept wings flows. The secondary stability of the former problem has already

been studied and it has been demonstrated that the most dangerous secondary mode has a large second harmonic component, a facet which has been observed in the work with J. P. Denier, concerning the most dangerous Görtler mode.

Work is continuing with P. Hall concerning the interaction of Görtler vortices and Rayleigh waves. The effect of a pressure gradient is being considered on the nonlinear development of high wavenumber vortices on a curved plate. The effect of compressibility is also being investigated. In this problem, suitable pressure gradients and Mach numbers imply that the underlying basic states contain inflection points and thus may support inviscid Rayleigh waves. The size of the waves may be such that although they remain linear themselves, they have a leading order effect on the basic flow. There is also some interaction with C. L. Streett (Theoretical Flow Physics Branch, LaRC) to investigate this phenomena with a linearised Navier-Stokes equations mentality, where selected nonlinear terms are retained that represent the vortex-wave interactions.

It is well known that as a Görtler vortex evolves downstream, its structure may be determined by a high wavenumber calculation. In this regime, it is known that the vortex boundaries are susceptible to wavy modes out of phase with the vortex state; this is similar to the wavy modes observed in the Taylor problem. Currently a study is being made to consider the nonlinear fate of these modes. This extends the previous linear and weakly nonlinear work.

Work has begun (which it is hoped will prove innovative) into a description of the noise that will emanate from an unsteady boundary layer. The particular problem that is discussed is a Rayleigh layer which arises when the fluid above a flat plate has an impulsive velocity imparted to it parallel to the plate. Using both Orr-Sommerfeld and triple deck methods, the resulting boundary layer has been shown to be unstable to Tollmien-Schlichting waves. It is conjectured that this wave will generate a sound field. In this case the radiated noise is likely to be small due to the spatial homogeneity of the problem in planes parallel to the plate; however, the solution may provide insight into the fully turbulent problem which may ensue.

#### J. Ray Ristorcelli

Fundamental issues involving the Reynolds stress modeling and computation of compressible turbulence in anisotropic and inhomogeneous situations are being investigated. The density flux emerges as an important quantity relating the compressible turbulence problem to the incompressible one in inhomogeneous flows. It is also an important quantity relating time-averaged and Favre-averaged statistics and is therefore relevant to the comparison of experimental and numerical results. Algebraic models for the density flux were derived from

its evolution equation. Key features of the model involve its dependence on the Reynolds stress which assures realizability. Current models are known to be very destabilizing and this problem can be linked to realizability violations. The model also shows a dependence of the density flux on the mean density and mean velocity gradient and other components of the density flux. The inclusion of the mean velocity gradient, which reflects more substantially the physics apparent from the evolution equation of the density flux, is anticipated to ameliorate boundedness issues in the transit through a shock. Testing of, and computations with the model are being conducted in coordination with R. Abid and T. Gatski using code developed for three-dimensional flows by J. Morrison.

Inadequacies and inconsistencies in the usual formulation of the mean and second-order equations typically used in the literature have been corrected. The reformulation of the viscous terms in the mean equations allows the mean flow equations to be carried without any modeling assumptions. The reformulation of the second-order equations is essential to the proper formulation of the near wall problem in low-Reynolds number models. Carrying the exact equations for the mean flow and the second-order statistics is expected to be important in complex flows: through shocks, near separation and in the viscous heated layer adjacent to the wall at high Mach number.

In the area of incompressible turbulence a rapid-pressure model frame-indifferent in the two-dimensional limit is being optimized. The 2DMFI model which is derived from first principles satisfying the mathematical constraints of realizability and geostrophy insures that the modeled equations are consistent with the Taylor-Proudman theorem. This is a an issue of substantial importance in the computation of any complex flows. The model was developed as part of the thesis of Ristorcelli (1991). The 2DMFI model, without any sacrifice of its mathematical rigourous underpinnings, has been calibrated to the asymptotic homogeneous shear.

#### Sutanu Sarkar

In the past six months, we have completed two projects. The first one has demonstrated the suitability of the hybrid DNS approach for the computation of sound radiated from isotropic turbulence. The computations show that that the acoustic efficiency of isotropic turbulence is much smaller than that observed in subsonic jet experiments. In the second project, G. Erlebacher and myself investigated compressibility effects on the statistical structure of the velocity gradient field. This study showed that although compressibility strongly affects the orientation properties of the pressure gradient vector, the eigenstructure of the solenoidal part of the velocity is relatively insensitive to compressibility.

#### John Shebalin

Research on compressible turbulent phenomena through direct numerical simulation of Navier-Stokes flows is continuing. The phenomena under investigation currently include 3-D gravitational collapse in molecular clouds. This is an interesting general problem as it involves the creation of large density gradients and strongly converging flows which are maintained by transferring gravitational potential energy into fluid and thermal energy. The numerical method used is a Fourier pseudospectral one with a logarithmic variable formulation of the basic equations where bulk viscosity is utilized to help keep density gradients well resolved.

Also, a computer code using a standard Fourier spectral method has been written, debugged, and is being used to study the ergodic properties of 3-D homogeneous Euler turbulence. A similar computer code is being developed to study the ergodic properties of ideal 3-D magnetohydrodynamic turbulence. Different time-integration algorithms are being used to determine their effects on the development of expected statistical behavior. This work is an extension of an earlier effort which studied ergodic properties in ideal 2-D turbulence (and saw apparent non-ergodicity in ideal 2-D homogeneous magnetohydrodynamic turbulence).

## Charles Speziale

Research has been conducted in collaboration with R. Abid (High Technology Corporation, LaRC) on second-order closure models of turbulence. Some pitfalls in the calibration of second-order closure models have been uncovered. In particular, it has been shown that the application of the normalization constraint to low-order approximations for the pressure-strain correlation leads to models that are badly calibrated for basic turbulent shear flows. This constraint should be relaxed in the formulation of such models. In addition, the performance of a variety of second-order closure models in homogeneous plane strain turbulence with a solid body rotation has been tested. Unlike in the companion problem of rotating shear flow, the models are fundamentally incapable of properly describing the cases with strong rotations where they erroneously predict a flow restabilization. This is due to the fact that the instability mechanism is more subtle (i.e., it involves resonance). Future research will be devoted to correcting this deficiency. Due to the strong analogy between rotation and curvature, the problem of rotating plane strain turbulence serves as a useful test case to gauge the performance of turbulence models for stagnation point flows where there is streamline curvature.

## Saleh Tanveer

During the period, progress has been made in several directions.

We conjecture that for a certain class of evolution problems that include the three dimensional incompressible Euler equations, generically, the processes of singularity formation and transformation is restricted to  $t=0^+$  when the spatial domain is extended to include the entire complex plane (or planes for multiple independent space variables). The location of formation of singularity or transformation of existing ones can be located simply by noting where a perturbation expansion for 0 < t << 1 becomes disordered. In particular, applying this to the Taylor-Green problem, leads one to conclude that the width of the analyticity strip scales as  $\ln \frac{1}{t}$  for small t, in accordance to direct numerical calculations (M. Brachet, private communication).

This conjecture, if true, presents a novel method of direct numerical computation of time evolving problems directly in the complex spatial domain. The advantage of this method is that it is expected to remove all sensitivity from the dynamics and allows one to explicitly follow singularities in the complex plane(s) and see whether or not it impinges the real domain in finite time. We expect its use in answering fundamental questions of entropy blow up for the 3-D Euler equations.

This algorithm has been very successful (Baker, Siegel, Tanveer (1993), submitted to J.F.M) for an evolution problem where there is no spontaneous generation of singularities (viscous displacement in a Hele-Shaw cell). We are in the process of applying this to the unit Atwood ratio Rayleigh-Taylor flow where singularities can be spontaneously generated in the unphysical complex plane (Tanveer, 1992). Further, generalization of this algorithm have been made for special cases for the three dimensional Euler equations. We do not have any concrete numerical results as yet.

We have also made progress on a more precise understanding of singularity formation in the Kelvin-Helmholtz problem. We (Cowley, Baker, Tanveer & Paige, to be submitted to J.F.M) find that the formation of singularities in the real domain after a finite time can be traced back to time  $t=0^+$  when the problem is extended to the complex plane.

## Siva Thangam

A new effort involving the analysis of turbulence models for the prediction of a wide range of separated flows was undertaken from analytical, computational and experimental point of view. The initial phase of this collaborative effort (involving M.Y. Hussaini and Ye Zhou of ICASE, Thomas Gatski of Theoretical Flow Physics Branch, S. Thangam of Stevens and George Vahala of William & Mary) was started with emphasis on the development of Reynolds stress closure models based on Renormalization Group Theory. During this period,

a formal representation for the Reynolds stress closure based on the recursive application of renormalization groups has been completed. During the next phase this model will be validated for a variety of separated flows from a computational point of view using a second-order accurate finite-volume algorithm.

In addition, during this period the third phase of the collaborative effort on the experimental and computational analysis of massively separated flows past a backward facing step (involving M.Y. Hussaini and S. Thangam of ICASE, and S.O. Kjelgaard of Experimental Methods Branch) was completed. The evaluation of two-equation Reynolds stress closure models based on a finite-volume algorithm and the new set of experimental data further verified the earlier findings which indicated that accurate prediction of the dominant features of the flow field, namely the size of the separation bubble, the mean velocity profiles, and the wall pressure variation is possible with anisotropic eddy-viscosity models. This work is to be continued by the Experimental Methods branch to develop a detailed experimental data base for channels of different step-to-channel height ratio for future efforts involving the validation of Reynolds stress closure models.

## Lu Ting

In collaboration with Drs. L. Maestrello and A. Frendi of NASA, we study a structural acoustic interaction problem which arises in the transmission of exterior incident waves through an airframe into the interior. The mathematical model simulates the experiments conducted at NASA. A flexible panel is mounted on a large rigid plate. Nearly planar waves are generated, incident normal to the plate at t=0. The incident wave frequency is near a natural frequency of the panel so that nonlinear oscillation of the panel can be excited. The real time pressure variations on the incident and transmitted sides are measured.

In our theoretical study of the scattering of an incident wave by a flexible panel, the panel vibration is governed by the nonlinear plate equation with the loading on the panel given by the pressure difference across the panel. The pressure difference requires the solution of the acoustic fields on both sides of the plate. This is an initial value problem since the panel oscillation is excited for t > 0. Two mathematical models are used to calculate this structural-acoustic interaction problem. One solves numerically the three dimensional nonlinear Euler equations for the flow field coupled with the plate equations (the fully coupled model). Approximate boundary conditions on the finite computational domain of the flow field are employed for the Euler solver. The second model uses the linear wave equation for the acoustic field and expresses the load as a double integral involving the panel oscillation (the decoupled model). The integral is an exact solution of the initial value problem for the acoustic field. The panel oscillation is then governed by a system of integro-differential

equations and is solved numerically. The acoustic field is then defined by an explicit formula, the double integral. Numerical results are obtained using the two models for linear and nonlinear panel vibrations. The predictions given by these two models are in good agreement but the computational time needed for the "fully nonlinear model" is 60 times longer than that for "the decoupled model". Detailed description of these two models and the numerical results will be presented in a forth coming ICASE report, entitled "An efficient model for coupling structural vibration with acoustic radiation", by A. Frendi, L. Maestrello and L. Ting.

#### Robert Wilson

Local mode analysis (LMA) was used to predict the smoothing properties and thus the efficiency of multigrid algorithms. The results from LMA were compared to practical smoothing factors by solving the flow over a backward facing step. In collaboration with A.O. Demuren, time-accurate codes are under development to solve free shear layer flows both laminar and turbulent, with the effect of unresolved scales being modeled by two-equation and Reynolds stress models (Reynolds averaged calculations) and subgrid-scale models (large eddy simulations).

#### Ye Zhou

In work done in collaboration with George Vahala, we have concentrated our efforts on the development of renormalization group based turbulence models. There are two distinctive RNG approaches of RNG to fluid turbulence: one called  $\epsilon$ -RNG, and the other called recursive-RNG. In particular, we point out here that in  $\epsilon$ -RNG, a small parameter  $\epsilon$  is introduced through the forcing correlation function. Yakhot & Orszag have to extrapolate from  $\epsilon \ll 1$  to  $\epsilon \to 4$  in order to reproduce the Kolmogorov energy spectrum. Furthermore, it is also necessary to take the distant interaction limit,  $k \to 0$ . In recursive RNG, The  $\epsilon$ -expansion is not applied. The turbulent transport coefficients are determined for the whole resolvable wavenumber scales.

We have applied the recursive RNG theory to develop the model for the Reynolds stress. It is well know that the traditional Boussinesq eddy viscosity model is deficient and several nonlinear Reynolds stress models have developed based on the direct interaction approximation (Yoshizawa) and  $\epsilon$ -RNG (Rubinstein and Barton). These model can be obtained simply on the ground of continuum mechanical (Speziale). The recursive RNG not only reproduced these terms, but also generated a novel triple product of mean velocity gradients. This term may play important role in the wall region. Currently, we are testing the model for the back step problem (with Thangam).

We have considered the advection of a passive scalar by incompressible turbulence using recursive renormalization group procedures in the differential subgrid shell thickness limit. It is shown explicitly that the higher order nonlinearities induced by the recursive renormalization group procedure preserve Galilean invariance. The recursive renormalization transport coefficients and the associated eddy Prandtl number are in good agreement with the k-dependent transport coefficients derived from closure theories and experiments.

#### APPLIED COMPUTER SCIENCE

#### Tom Crockett

A preliminary version of a portable parallel graphics library for message-passing architectures is now operational on the Intel iPSC/860. The library will serve both as a vehicle for continuing research in parallel rendering algorithms, and as a base for developing parallel visualization methods. A sequential version of the library also runs on Sun and SGI workstations.

The graphics library incorporates a new parallel renderer derived from the original Orloff/Crockett algorithm. The new renderer is based on spans rather than trapezoids, which provides improved scalability and more flexibility in load balancing. Initial, untuned performance measurements indicate parallel efficiencies and rendering rates that are approximately double that of the original parallel renderer, even with the inclusion of substantial new functionality.

In joint work, Bokhari, Crockett, and Nicol developed a new graph partitioning method known as Parametric Binary Dissection (PBD), and an optimized variant called Fast Dissection. In adapting these techniques for use in color image quantization, improvements have been made which take into account properties of the regions to decide which region to cut next and in which direction. For color quantization, this results in reduced color error. For other applications, such as partitioning unstructured grids, the same techniques might result in improved load-balancing characteristics. This is an area for future investigation.

A draft of a visualization research plan for ICASE was developed in the late Fall. The plan takes into account visualization needs within ICASE and in several of the principal computational branches throughout Langley Research Center. This plan will be gradually implemented in the coming months as additional visualization staff arrives.

#### Phil Dickens

CSIM is a widely used simulation package based on the C programming language. Currently, CSIM is implemented on several workstations including a Sun-3, Sun-4, Vax, IBM RS6000 and HP 300, as well as various personal computers. The problem is that these workstations and personal computers are often not powerful enough to efficiently run many of the large simulation programs which use CSIM. In order to meet the computational demands of these large simulations we are designing a multiprocessor implementation of CSIM for the Intel I860, the Intel Paragon and for a network of workstations using PVM. This work is in collaboration with David Nicol and Cathy Roberts.

In addition to our work on a multiprocessor design for CSIM we have continued our investigation of parallel simulation protocols which blend aspects of aggressive and non-aggressive approaches. This research is in collaboration with David Nicol, Paul Reynolds, Jr. (Department of Computer Science, University of Virginia), and Mark Duva (Department of Applied Mathematics, University of Virginia). We have developed an analytic model to predict the expected improvement in performance as aggressiveness is added to a non-aggressive windowing protocol. Our research has shown that if the cost of saving state is not too high, or if the cost of global synchronization is large, the benefits of extending the conservative simulation window exceeds the costs, and better performance than that achieved by the non-aggressive approach is possible. Simulation studies support the results of our model.

#### Ulf Hanebutte

Work was started on parallelizing the adaptive mesh refinement algorithm (AMR) developed within ICASE by Quirk. The AMR algorithm belongs to a complex class of schemes that have proven to be highly successful on both vector and serial machines for simulating transient flow phenomena which contain disparate length and time scales. Whilst such algorithms exhibit a high degree of parallelism at a conceptual level, it remains to be seen whether they can exploit current parallel architectures. Specifically, the AMR algorithm cannot be reduced to a small kernel upon which various parallelizing strategies could be tested. Therefore the development of a parallel AMR algorithm is a non-trivial exercise which necessitates the creation of an elaborate framework before individual components can be parallelized. However, since the AMR algorithm has been shown to be applicable to a wide class of problems, much if not all of this framework will be required by future projects, and hence this initial development work should not be viewed as effort wasted.

Thus far we have identified a parallelizing strategy which will preserve the basic structure of the serial algorithm and so it should also retain the proven generality of the original serial code. This strategy relies only on the existence of some standard message passing methodology and so portability between a broad class of parallel computers should be expected. This should also ensure a long life time of the algorithm. Issues such as data distribution, file I/O and compatibility of the stored data between new parallel and the original serial code have been addressed. Major modules of the initial parallel framework have been designed and are currently being implemented. The parallel virtual machine (PVM) environment utilizing the ICASE computer facilities is being used for the initial development and testing of the parallel algorithm.

Lastly, whilst by their very nature dynamic adaptive algorithms present load balance difficulties, many physical problems of real interest have features which lead naturally to an acceptable load balance. Consequently one can solve real class problems even during the stages of the of the parallel code development. In the near future we hope to be able to perform detailed simulations of detonation waves with the aim of predicting, quantitatively, detonation cell sizes; a task that has hitherto met with little success largely due to insufficient computing power.

# David Keyes

Demands for massive memory and high speed typically accompany one another in scientific and engineering computations, linking space and time in algorithm design. When memory requirements are small or time is not at a premium, algorithms can be designed without regard for data access patterns; otherwise, some degree of control must be exerted over data layout. This general imperative becomes more important in programming the scalable distributed memory machines from which the earliest useful teraflops are expected. Fortunately, the laws of nature often cooperate with a basic scaling law of computer architecture: The magnitude of interaction between two degrees of freedom in a physical system decays with their spatial separation; therefore, the frequency and volume of data exchange between different points in the computational domain can be allowed to decay with distance without sacrifice of algorithmic optimality. For model problems, this simple intuition can be formalized in convergence theorems.

Modern iterative domain decomposition (or "substructuring") methods require predominantly local information. Nonlocal information is accessed hierarchically, through exchanges requiring only a small volume of data relative to the scale of the discretization. Hence, domain decomposition is an natural algorithmic bridge between application and architecture for elliptically dominated problems, such as inverting the left-hand sides of deferred-correction methods for aerodynamic steady states. We have replaced conventional approximation solvers in compressible Euler codes with parallel implicit domain decomposition solvers, which permits large CFL numbers without time factorization error. Since the domain decomposition solvers are more expensive per step, work continues on improving their preconditioning ability and on better control algorithms for adapting the CFL number to exploit such a fully implicit solver.

# Scott Leutenegger

In collaboration with Dan Dias from IBM T.J. Watson Research Center, we have conducted a modelling study of the TPC-C benchmark for both single node and distributed

database management systems. We simulated the TPC-C workload to determine expected buffer miss rates assuming an LRU buffer management policy. These miss rates are then used as inputs to a throughput model. From these models we show the following: (i) We quantify the data access skew as specified in the benchmark and show what fraction of the accesses go to what fraction of the data. (ii) We quantify the resulting buffer hit ratios for each relation as a function of buffer size. (iii) We show that close to linear scale-up (about 3% from the ideal) can be achieved in a distributed system, assuming replication of a read-only table. (iv) We examine the effect of packing hot tuples into pages and show that significant price/performance benefit can be thus achieved. (v) Finally, by coupling the buffer simulations with the throughput model, we examine typical disk/memory configurations that maximize the overall price/performance. Results from this study will be presented at SIGMOD 93.

In collaboration with Xian-He Sun, we have investigated the use of distributed computing in a non-dedicated environment. The high cost of current multiprocessor machines and the availability of clusters of workstations have lead researchers to re-explore distributed computing using independent workstations for parallel processing. This distributed computing approach may provide better cost/performance than high performance multiprocessor machines. In addition, a distributed computing approach can utilize the wasted cycles of idle workstations for speeding up or scaling large computations. In a non-dedicated environment, workstation owner's processes compete with parallel program tasks for cycles. We have addressed the feasibility of using such a non-dedicated system for execution of parallel computations assuming workstation processes have preemptive priority over parallel tasks. We have developed an analytical model to predict parallel job response times assuming this non-dedicated system. By using this model, we provide insight into how significantly workstation owner interference degrades parallel program performance. We have introduced a new metric which we call the task ratio, which relates the parallel task demand to the mean service demand of non parallel workstation processes. We propose that the task ratio is a useful metric for determining how large the demand of a parallel applications must be in order to make efficient use of a non-dedicated distributed system. This metric for non-dedicated systems may be just as important as the communication/computation ratio.

#### Piyush Mehrotra

A large percentage of scientific applications exhibit data parallelism. Partially based on work done at ICASE on the languages Kali and Vienna Fortran, an international group of researchers has designed High Performance Fortran (HPF). The main aim of HPF is to provide a standard set of distribution directives to exploit data parallelism in scientific codes.

However, it is clear that HPF does not have enough expressive power to specify the distributions required for a large number of codes. We have been investigating the limitations of HPF when applied to NASA codes. One area of focus is block-structured grids codes. In an joint effort with John Van Rosendale, we have used the Vienna Compiler system to study several multi-block codes (in particular LARCK and CMG). The fundamental issue in such codes is to distribute the data such that the individual grid blocks are spread over subsets of processors. HPF currently does not provide such a capability and has to be extended to provide this finer degree of control. Beyond expressing such distributions, we are also working on compiler technology to recognize and exploit both the inter-grid and the intra-grid parallelism present in such codes.

In a joint effort with Mike Cokus and John Van Rosendale, we have been studying the optimizing of communication for unstructured computations. In previous work, we have exploited the inspector/executor paradigm to generate communication patterns for irregular computations at runtime. We have designed a set of directives which allow the user to control the saving and reuse of such communication patterns. Using such directives, the user can specify, for example that the communication patterns for the grids at different levels in an unstructured multigrid code, to be saved when first generated in a procedure and reused when the same procedure is recalled with the same grid.

Jointly with John Van Rosendale, Barbara Chapman and Hans Zima, we have been studying the mechanisms for pushing the state-of the art in HPF-related languages and compiler design. One area is the study of self-scheduled parallel loops which would allow work-queue kind of paradigms to be exploited in the context of HPF. We have also been investigating the use of task parallelism in scientific codes. The goal is to provide an environment which allows multiple kinds of parallelism (task and data in particular) to be exploited together within the same code.

#### David Nicol

In collaboration with Weizhen Mao (William & Mary), I investigated the problem of optimally scheduling communication on a toroidally connected SIMD parallel architecture. We find that if the architecture can use all communication ports simultaneously, and if the application's communication requirements are identical at every PE, then a low-order polynomial time algorithm exists to find the optimal schedule.

In collaboration with Dan Palumbo (NASA LaRC), I refined a reliability estimation tool, ASSURE, to include an option for automated parallelization across a local area network, and to include an option for monte carlo (rather than exact) analysis. These refinements serve to accelerate the solution time of ASSURE models considerably.

In collaboration with Phil Heidelberger (IBM Research), I studied the performance of parallel simulations that synchronize on the basis of uniformized communication schedules. Several variations of the algorithm were analyzed.

In collaboration with Richard Fujimoto (Georgia Tech), I wrote a state-of-the-art survey on parallel simulation.

Finally, I developed a new automated mapping algorithm for parallel discrete-event simulations, and incorporated it into a parallel simulation of timed Petri nets. The algorithm provably finds the optimal mapping on a large class of regular problems. Combined with dynamic remapping policies, the method very effectively reduces the runtime of parallel discrete event simulations.

# Matthew Rosing

Work in developing a low latency message interface and compiler techniques for the efficient use of distributed memory machines continues.

A prototype compiler was built to support user defined compile time functions. The language provides the ability for compiler modules to be easily added to the base language, Fortran. A prototype module that supports Fortran90-like array operations, distributed data, and high level message based communications was also built. The time to build the module was approximately three weeks. This relatively short time to add constructs to a language indicates the viability of using domain specific modules to more easily develop efficient applications.

A portable low latency communication interface for distributed memory multiprocessors has been defined. The model is based on having both a computation and communication processor on each node. Communications consists of sending either code or data between nodes. Code is executed by the communication processor and data can be read by either processor. This limited amount of parallelism more efficiently supports overlapping communication and computation and also utilizes node resources more efficiently.

#### Joel Saltz

I am designing tools to characterize the performance of structured adaptive and adaptive unstructured codes. The performance characteristics of these codes are complex functions of dynamically changing communications costs and load imbalances. I plan to create the facilities for presenting performance data in the context of the high level programming language in which the program was written. For example, my group at Maryland has developed, in collaboration with G. Fox, a prototype (extended) HPF compiler able to generate code for

a range of unstructured and block structured problems. The new performance tools would combine performance timings obtained through instrumenting generated code with data layout and geometrical information specified by the users extended HPF program. This tool will produce a graphical display of communication and load balance information that is presented in the context of the programmer specified data layout and geometrical information.

# Hong Zhang Sun

The waveform multigrid method is a time-parallel method for solving certain type of time-dependent partial differential equations. In collaboration with Shlomo Ta'asan, we performed a Fourier-Laplace analysis of the convergence rate of the sequential version of this algorithm, which provided significant insight into the method. We have also investigated the relationship between the waveform multigrid method for time-dependent problems and the analogous multigrid method for steady-state problems. Based on our investigations, we have been able to accurately predict the performance of the algorithm for time-dependent problems. We have shown that the convergence rate of the time-parallel algorithm is essentially the same as that for the standard steady-state multigrid algorithms. The numerical experiments we have performed confirm our analytical results. The next step is to design a parallel waveform multigrid algorithm for nonlinear time-dependent problems and implement it on a parallel machine. Some real applications are under consideration.

The joint work with V. Ervin (Clemson University) and W. Layton (University of Pittsburgh) on the generalized alternating direction implicit method is continuing. Some parameter dependencies have been observed and are under investigation.

#### Xian-He Sun

A central goal of parallel processing is to achieve better, more accurate solutions. One requirement for obtaining a more accurate solution is to adopt discretization methods with high-order accuracy. Previously, a highly accurate discretization scheme, the compact finite-difference scheme, has been proposed. However, the almost symmetric Toeplitz tridiagonal systems that arise from compact schemes are sequential in nature and difficult to solve efficiently on parallel computers. In recent study, I have introduced a parallel algorithm, the simple parallel prefix (SPP) algorithm, for compact schemes.

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The SPP algorithm is designed for fine-grain computing. With n processors, the SPP algorithm solves an n-dimensional system with  $2\log(n) + 1$  AXPY operations. Two prefix communications are required in the solving phase and one broadcast communication is required in the modification phase. In comparison with existing parallel solvers, the SPP algorithm is simple in computing and simple in communication. It requires storage of only

one  $\log(n)$ -dimensional vector for the computing phase and one n-dimensional vector for the modification phase. When the tridiagonal system is diagonally dominant, both the computing and the modification phases can be truncated without degrading the accuracy. Memory requirements will be further reduced when truncation is applied. A detailed accuracy analysis has been conducted to find the appropriate truncation number. Experimental results show that the SPP algorithm achieves a speedup greater than 1500 over the best sequential algorithm on a 16K PEs MasPar M-1 SIMD parallel computer. In addition to the good performance on the SIMD machines, the SPP algorithm also out performs the best sequential algorithm on a vector machine (Cray 2), even on systems with multiple right sides. Experimental and theoretical results show that the SPP algorithm is a good choice for compact schemes and for the emerging high-performance parallel computers.

The SPP algorithm is a continuation of efforts to design efficient parallel solvers for compact scheme. An efficient solver, the PDD algorithm, for coarse- or median-grain computing has been proposed previously. The PDD algorithm and the SPP algorithm can be combined on parallel machines with vector processing units.

#### John Van Rosendale

While mapping of standard multigrid to parallel architectures has been well studied, new issues arise in mapping more complex multigrid algorithms. Algorithms based on line- or plane-relaxation, or algorithms using multiple semicoarsened grids (MSG algorithms) are needed for problems having stretched grids or anisotropic operators. Mapping these algorithms to parallel architectures is challenging, because of the large amount of communication required and the complex load balancing issues arising. Parallel implementation of these algorithm is important in many applications areas, including computational fluid dynamics.

In collaboration with Andrea Overman of the Computational Sciences branch, we are currently studying the issues involved in mapping MSG (multiple semicoarsened grid) multigrid to scalable memory machines like the Intel Paragon. One version of this algorithm uses standard V-cycle multigrid, in which the smoothing iteration is done on only one multigrid level at a time. This is an effective numerical algorithm, but raises difficult mapping issues on distributed memory architectures. There is also a more parallel version of this algorithm, using a C-cycle in which all levels are smoothed simultaneously. The latter is simpler to map to parallel machines, but does not appear to be as efficient. We are currently exploring several approaches to mapping the V-cycle algorithm to parallel machines, like the Paragon, and are also looking at improving the performance of the simpler C-cycle version.

#### Mohammed Zubair

In this research, we are focusing on the design of algorithms for numerically intensive kernels commonly encountered in large scientific computations arising out of NASA applications. These algorithms are being designed for various distributed memory parallel machines.

The availability of basic computational kernels will help in porting existing applications or implementing new NASA applications on parallel machines. These kernels will be tuned to a particular architecture and will result in an efficient implementation of the complete application. Thus a scientist or an engineer wishing to perform massively parallel computations need not be aware of various hardware/software features of a parallel machine that are critical for obtaining good performance.

One of the kernels which we are investigating is the three-dimensional FFT kernel. We have integrated the 3-D FFT kernel with the three dimensional DNS code. We are currently testing and evaluating the performance of the complete code on the Intel iPSC/860 machine. Besides FFT, this code has several other computational intensive kernels such as penta-diagonal solvers, matrix-matrix multiplier, etc. The 3-dimensional data mapping determines which of the kernel needs to be parallelized. In our first attempt we have mapped the three dimensional (x-y-z) data with a number of xy-planes getting mapped to a node of the Intel iPSC/860. This mapping requires parallelization of the FFT kernel. The rest of the kernels are executed locally.

#### REPORTS AND ABSTRACTS

Mavriplis, Dimitri: An advancing front Delaunay triangulation algorithm designed for robustness. ICASE Report No. 92-49, October 15, 1992, 32 pages. Submitted to Journal of Computational Physics.

A new algorithm is described for generating an unstructured mesh about an arbitrary two-dimensional configuration. Mesh points are generated automatically by the algorithm in a manner which ensures a smooth variation of elements, and the resulting triangulation constitutes the Delaunay triangulation of these points. The algorithm combines the mathematical elegance and efficiency of Delaunay triangulation algorithms with the desirable point placement features, boundary integrity, and robustness traditionally associated with advancing-front-type mesh generation strategies. The method offers increased robustness over previous algorithms in that it cannot fail regardless of the initial boundary point distribution and the prescribed cell size distribution throughout the flow-field.

Shebalin, John V.: Homogeneous quantum electrodynamic turbulence. <u>ICASE Report No. 92-50</u>, October 7, 1992, 28 pages. Submitted to Physica D.

The electromagnetic field equations and Dirac equations for oppositely charged wave functions are numerically time-integrated using a spatial Fourier method. The numerical approach used, a spectral transform technique, is based on a continuum representation of physical space. The coupled classical field equations contain a dimensionless parameter which sets the strength of the nonlinear interaction (as the parameter increases, interaction volume decreases). For a parameter value of unity, highly nonlinear behavior in the time-evolution of an individual wave function, analogous to ideal fluid turbulence, is observed. In the truncated Fourier representation which is numerically implemented here, the quantum turbulence is homogeneous but anisotropic and manifests itself in the nonlinear interacting fermionic wave functions quickly approach a multi-mode, dynamic equilibrium state, and that this state can be determined by numerical means.

Nicol, David, Rahul Simha, and Don Towsley: Static assignment of complex stochastic tasks using stochastic majorization. ICASE Report No. 92-51, October 8, 1992, 24 pages. Submitted to Journal of Parallel and Distributed Computing.

We consider the problem of statically assigning many tasks to a (smaller) system of homogeneous processors, where a task's structure is modeled as a branching process, and all tasks are assumed to have identical behavior. We show how the theory of majorization can be used to obtain a partial order among possible task assignments. Our results show that if the vector of numbers of tasks assigned to each processor under one mapping is majorized by that of another mapping, then the former mapping is better than the latter with respect to a large number of objective functions. In particular, we show how measurements of finishing time, resource utilization, and reliability are all captured by the theory. We also show how the theory may be applied to the problem of partitioning a pool of processors for distribution among parallelizable tasks.

Lighthill, James: A general introduction to aeroacoustics and atmospheric sound. ICASE Report No. 92-52, October 9, 1992, 34 pages. To appear in Proceedings of the ICASE/NASA LaRC Workshop on Computational Aeroacoustics held April 6-9, 1992.

This paper uses a single unifying principle (based upon the nonlinear "momentum-flux" effects produced when different components of a motion transport different components of its momentum) to give a broad scientific background to several aspects of the interaction between airflows and atmospheric sound. First, it treats the generation of sound by airflows of many different types. These include, for example, jet-like flows involving convected turbulent motions – with the resulting aeroacoustic radiation sensitively dependent on the Mach number of convection – and they include, as an extreme case, the supersonic "boom" (shock waves generated by a supersonically convected flow pattern). Next, the paper analyses sound propagation through nonuniformly moving airflows, and quantifies the exchange of energy between flow and sound; while, finally, it turns to problems of how sound waves "on their own" may generate the airflows known as acoustic streaming.

Lighthill, James: Report on the final panel discussion on computational aeroacoustics. ICASE Report No. 92-53, October 9, 1992, 14 pages. To appear in Proceedings of the ICASE/NASA LaRC Workshop on Computational Aeroacoustics held April 6-9, 1992.

This paper by the Panel Chairman summarises some important conclusions about future prospects for aeroacoustics in general, and for computational aeroacoustics in particular, that were reached in the course of the Final Panel Discussion of the Workshop on Computational Aeroacoustics held from 6 to 9 April 1992 by ICASE and NASA Langley Research Center.

Tanveer, S. and C.G. Speziale: Singularities of the Euler equation and hydrodynamic stability. ICASE Report No. 92-54, October 9, 1992, 22 pages. Submitted to Physics of Fluids A.

Equations governing the motion of a specific class of singularities of the Euler equation in the extended complex spatial domain are derived. Under some assumptions, it is shown how this motion is dictated by the smooth part of the complex velocity at a singular point in the unphysical domain. These results are used to relate the motion of complex singularities to the stability of steady solutions of the Euler equation. A sufficient condition for instability is conjectured. Several examples are presented to demonstrate the efficacy of this sufficient condition which include the class of elliptical flows and the Kelvin-Stuart Cat's Eye.

Harten, Ami, and Itai Yad-Shalom: Fast multiresolution algorithms for matrix-vector multiplication. ICASE Report No. 92-55, October 15, 1992, 43 pages. Submitted to SIAM Journal of Numerical Analysis.

In this paper we present a class of multiresolution algorithms for fast application of structured dense matrices to arbitrary vectors, which includes the fast wavelet transform of Beylkin, Coifman and Rokhlin and the multilevel matrix multiplication of Brandt and Lubrecht. In designing these algorithms we first apply data compression techniques to the

matrix and then show how to compute the desired matrix-vector multiplication from the compressed form of the matrix. In describing this class we pay special attention to an algorithm which is based on discretization by cell-averages as it seems to be suitable for discretization of integral transforms with integrably singular kernels.

Dubey, A., M. Zubair, and C.E. Grosch: A general purpose subroutine for fast Fourier transform on a distributed memory parallel machine. ICASE Report No. 92-56, November 13, 1992, 14 pages. Submitted to International Conference on Mathematical Modelling & Scientific Computing, Dec. 7-11, 1992, Bangalore.

One issue which is central in developing a general purpose FFT subroutine on a distributed memory parallel machine is the data distribution. It is possible that different users would like to use the FFT routine with different data distributions. Thus there is a need to design FFT schemes on distributed memory parallel machines which can support a variety of data distributions. In this paper we present an FFT implementation on a distributed memory parallel machine which works for a number of data distributions commonly encountered in scientific applications. We have also addressed the problem of rearranging the data after computing the FFT. We have evaluated the performance of our implementation on a distributed memory parallel machine Intel iPSC/860.

Speziale, C.G., R.M.C. So, and B.A. Younis: On the prediction of turbulent secondary flows. ICASE Report No. 92-57, October 15, 1992, 21 pages. To appear in Near-Wall Turbulent Flows, Elsevier Press.

The prediction of turbulent secondary flows with Reynolds stress models in circular pipes and non-circular ducts is reviewed. Turbulence-driven secondary flows in straight non-circular ducts are considered along with turbulent secondary flows in pipes and ducts that arise from curvature or a system rotation. The physical mechanisms that generate these different kinds of secondary flows are outlined and the level of turbulence closure required to properly compute each type is discussed in detail. Illustrative computations of a variety of different secondary flows obtained from two-equation turbulence models and second-order closures are provided to amplify these points.

Gatski, T.B., and C.G. Speziale: On explicit algebraic stress models for complex turbulent flows. ICASE Report No. 92-58, November 13, 1992, 34 pages. To be submitted to the Journal of Fluid Mechanics.

Explicit algebraic stress models that are valid for three-dimensional turbulent flows in non-inertial frames are systematically derived from a hierarchy of second-order closure models. This represents a generalization of the model derived by Pope [J. Fluid Mech. 72, 331 (1975)] who based his analysis on the Launder, Reece and Rodi model restricted to two-dimensional turbulent flows in an inertial frame. The relationship between the new models and traditional algebraic stress models – as well as anistropic eddy viscosity models – is theoretically established. The need for regularization is demonstrated in an effort to explain why traditional algebraic stress models have failed in complex flows. It is also shown that

these explicit algebraic stress models can shed new light on what second-order closure models predict for the equilibrium states of homogeneous turbulent flows and can serve as a useful alternative in practical computations.

Sun, Xian-He, and Lionel M. Ni: Scalable problems and memory-bounded speedup. ICASE Report No. 92-59, November 17, 1992, 23 pages. Submitted to Journal of Parallel and Distributed Computing.

In this paper three models of parallel speedup are studied. They are fixed-size speedup, fixed-time speedup and memory-bounded speedup. The latter two consider the relationship between speedup and problem scalability. Two sets of speedup formulations are derived for these three models. One set considers uneven workload allocation and communication overhead, and gives more accurate estimation. Another set considers a simplified case and provides a clear picture on the impact of the sequential portion of an application on the possible performance gain from parallel processing. The simplified fixed-size speedup is Amdahl's law. The simplified fixed-time speedup is Gustafson's scaled speedup. The simplified memory-bounded speedup contains both Amdahl's law and Gustafson's scaled speedup as special cases. This study leads to a better understanding of parallel processing.

Nicol, David M., and Philip Heidelberger: Parallel algorithms for simulating continuous time Markov chains. ICASE Report No. 92-60, November 18, 1992, 23 pages. Submitted to the 7th Annual Workshop on Parallel and Distributed Simulation.

We have previously shown that the mathematical technique of uniformization can serve as the basis of synchronization for the parallel simulation of continuous-time Markov chains. This paper reviews the basic method and compares five different methods based on uniformization, evaluating their strengths and weaknesses as a function of problem characteristics. The methods vary in their use of optimism, logical aggregation, communication management, and adaptivity. Performance evaluation is conducted on the Intel Touchstone Delta multiprocessor, using up to 256 processors.

Shebalin, John V.: Pseudospectral simulation of compressible turbulence using logarithmic variables. ICASE Report No. 92-61, November 25, 1992, 20 pages. Submitted to the 11th AIAA Computational Fluid Dynamics Meeting on July 6-9, 1992, at Orlando, FL.

The direct numerical simulation of dissipative, highly compressible turbulent flow is performed using a pseudospectral Fourier technique. The governing equations are cast in a form where the important physical variables are the fluid velocity and the natural logarithms of the fluid density and temperature. Bulk viscosity is utilized to model polyatomic gases more accurately and to ensure numerical stability in the presence of strong shocks. Numerical examples include three-dimensional supersonic homogeneous turbulence and two-dimensional shock-turbulence interactions.

Nicol, David, and Richard Fujimoto: Parallel simulation today. ICASE Report No. 92-62, November 25, 1992, 36 pages. To appear in Annals of Operation Research.

This paper surveys topics that presently define the state of the art in parallel simulation. Included in the tutorial are discussions on new protocols, mathematical performance analysis, time parallelism, hardware support for parallel simulation, load balancing algorithms, and dynamic memory management for optimistic synchronization.

Berger, S.A., and G. Erlebacher: Vortex breakdown incipience: Theoretical considerations. ICASE Report No. 92-63, November 27, 1992, 26 pages. To be submitted to Theoretical & Computational Fluid Dynamics.

The sensitivity of the onset and the location of vortex breakdowns in concentrated vortex cores, and the pronounced tendency of the breakdowns to migrate upstream have been characteristic observations of experimental investigations; they have also been features of numerical simulations and led to questions about the validity of these simulations. This behavior seems to be inconsistent with the strong time-like axial evolution of the flow, as expressed explicitly, for example, by the quasi-cylindrical approximate equations for this flow. An order-of-magnitude analysis of the equations of motion near breakdown leads to a modified set of governing equations, analysis of which demonstrates that the interplay between radial inertial, pressure, and viscous forces gives an elliptic character to these concentrated swirling flows. Analytical, asymptotic, and numerical solutions of a simplified non-linear equation are presented; these qualitatively exhibit the features of vortex onset and location noted above.

Quirk, James J.: A contribution to the great Riemann solver debate. ICASE Report No. 92-64, November 27, 1992, 33 pages. Submitted to International Journal for Numerical Methods in Fluids.

The aims of this paper are threefold: to increase the level of awareness within the shock capturing community to the fact that many Godunov-type methods contain subtle flaws that can cause spurious solutions to be computed; to identify one mechanism that might thwart attempts to produce very high resolution simulations; and to proffer a simple strategy for overcoming the specific failings of individual Riemann solvers.

Stott, Jillian A. K., and Peter W. Duck: The stability of a trailing-line vortex in compressible flow. ICASE Report No. 92-65, December 4, 1992, 54 pages.

We consider the inviscid stability of the Batchelor (1964) vortex in a compressible flow. The problem is tackled numerically and also asymptotically, in the limit of large (azimuthal and streamwise) wavenumbers, together with large Mach numbers. The nature of the solution passes through different regimes as the Mach number increases, relative to the wavenumbers. At very high wavenumbers and Mach numbers, the mode which is present in the

incompressible case ceases to be unstable, whilst a new "centre mode" forms, whose stability characteristics are determined primarily by conditions close to the vortex axis. We find that generally the flow becomes less unstable as the Mach number increases, and that the regime of instability appears generally confined to disturbances in a direction counter to the direction of the rotation of the swirl of the vortex.

Throughout the paper comparison is made between our numerical results and results

obtained from the various asymptotic theories.

Banks, H.T., and R.C. Smith: The modeling of piezoceramic patch interactions with shells, plates and beams. ICASE Report No. 92-66, December 4, 1992, 32 pages. Submitted to Quarterly of Applied Mathematics.

General modes describing the interactions between a pair of piezoceramic patches and elastic substructures consisting of a cylindrical shell, plate and beam are presented. In each case, the manner in which the patch loads enter both the strong and weak forms of the time-dependent structural equations of motion is described. Through force and moment balancing, these loads are then determined in terms of material properties of the patch and substructure (thickness, elastic properties, Poisson ratios), the geometry of the patch placement, and the voltages into the patches. In the case of the shell, the coupling between bending and inplane deformations, which is due to the curvature, is retained. These models are sufficiently general to allow for potentially different patch voltages which implies that they can be suitably employed when using piezoceramic patches for controlling system dynamics when both extensional and bending vibrations are present.

Frendi, Abdelkader, Lucio Maestrello, and Alvin Bayliss: Coupling between plate vibration and acoustic radiation. ICASE Report No. 92-67, December 8, 1992, 37 pages. Submitted to Journal of Sound and Vibration.

A detailed numerical investigation of the coupling between the vibration of a flexible plate and the acoustic radiation is performed. The nonlinear Euler equations are used to describe the acoustic fluid while the nonlinear plate equation is used to describe the plate vibration. Linear, nonlinear, and quasi-periodic or chaotic vibrations and the resultant acoustic radiation are analyzed. We find that for the linear plate response, acoustic coupling is negligible. However, for the nonlinear and chaotic responses, acoustic coupling has a significant effect on the vibration level as the loading increases. The radiated pressure from a plate undergoing nonlinear or chaotic vibrations is found to propagate nonlinearly into the far-field. However, the nonlinearity due to wave propagation is much weaker than that due to the plate vibrations. As the acoustic wave propagates into the far-field, the relative difference in level between the fundamental and its harmonics and subharmonics decreases with distance.

Mavriplis, D.J., Raja Das, Joel Saltz, and R.E. Vermeland: Implementation of a parallel unstructured Euler solver on shared and distributed memory architecture. ICASE Report No. 92-68, December 9, 1992, 20 pages. Submitted to the Journal of Supercomputing.

An efficient three dimensional unstructured Euler solver is parallelized on a Cray Y-MP C90 shared memory computer and on an Intel Touchstone Delta distributed memory computer. This paper relates the experiences gained and describes the software tools and hardware used in this study. Performance comparisons between the two differing architectures are made.

Demuren, A.O., and R.V. Wilson: Estimating uncertainty in computations of two-dimensional separated flows. ICASE Report No. 92-69, December 9, 1992, 32 pages. Submitted to ASME, Journal of Fluids Engineering.

The present paper investigates sources of uncertainties in two-dimensional flow computations and presents methods for estimating them. Two sample problems are used for illustration. The following categories are explored in detail: i.) Uncertainty due to truncation error in numerical schemes; ii.) Uncertainty due to discretization error; iii.) Uncertainty due to outflow boundary conditions; iv.) Uncertainty due to incomplete iterative convergence; v.) Uncertainty due to computational grid aspect ratio. The error estimates are based on requirements for internal consistencies in computed results. Therefore, they provide better judgement of the numerical solution integrity than comparisons to experimental data or "benchmark" solutions whose reliability may sometimes be questionable. Ideally, both approaches should be employed. New results are presented on the optimum grid-cell aspect ratio for computational accuracy and efficiency.

Dhanak, Manhar R.: Instability of flow in a streamwise corner. ICASE Report No. 92-70, December 18, 1992, 17 pages. Submitted to Proc. Roy. Soc. London A.

The linear stability of an incompressible laminar flow in the blending boundary layer between the boundary layer in a 90° streamwise corner and a Blasius boundary layer well away from the corner is examined using a locally parallel flow approximation. It is shown that the influence of the outer boundary conditions associated with oblique modes of disturbances which are anti-symmetric about the bisector plane have a profound effect on the stability of the flow. As a result, in good agreement with observation, the critical streamwise Reynolds number, associated with a spanwise location is significantly reduced as the corner is approached, being  $R_{cr} = 60$  approximately for spanwise distance of  $z^* = 6x^*R^{-1}$  from the corner compared with  $R_{cr} = 322$  approximately for  $z^* = 20x^*R^{-1}$ , where  $x^*$  measures downstream distance from the leading edges. At R = 600, the growth rate of the most amplified mode of disturbance at the former location is over six times greater than that at the latter; the corresponding wave angle at the two locations is respectively 44° and 5°, approximately.

Trefethen, Lloyd N., Anne E. Trefethen, Satish C. Reddy, and Tobin A. Driscoll: A new direction in hydrodynamic stability: Beyond Eigenvalues. ICASE Report No. 92-71, December 18, 1992, 31 pages. Submitted to Science.

Fluid flows that are smooth at low speeds become unstable and then turbulent at higher speeds. This phenomenon has traditionally been investigated by linearizing the equations of flow and looking for unstable eigenvalues of the linearized problem, but the results agree poorly in many cases with experiments. Nevertheless, it has become clear in recent years that linear effects play a central role in hydrodynamic instability. A reconciliation of these findings with the traditional analysis can be obtained by considering the "pseudospectra" of the linearized problem, which reveal that small perturbations to the smooth flow in the form of streamwise vortices may be amplified by factors on the order of 10<sup>5</sup> by a linear mechanism, even though all the eigenmodes are stable. The same principles apply also to other problems in the mathematical sciences that involve non-orthogonal eigenfunctions.

Bertolotti, Fabio P., and Jeffrey D. Crouch: Simulation of boundary-layer transition: Receptivity to spike stage. ICASE Report No. 92-72, December 21, 1992, 20 pages. To be submitted to Physics of Fluids.

The transition to turbulence in a boundary layer over a flat plate with mild surface undulations is simulated using the parabolized stability equations (PSE). The simulations incorporate the receptivity, the linear growth, and the nonlinear interactions leading to breakdown. The nonlocalized receptivity couples acoustic perturbations in the free stream with disturbances generated by the surface undulations to activate a resonance with the natural eigenmodes of the boundary layer. The nonlinear simulations display the influence of the receptivity inputs on transition. Results show the transition location to be highly sensitive to the amplitudes of both the acoustic disturbance and the surface waviness.

Geer, James F., and Dennis S. Pope: A multiple scales approach to sound generation by vibrating bodies. ICASE Report No. 92-73, December 22, 1992, 45 pages. To be submitted to Journal of Fluid Mechanics.

The problem of determining the acoustic field in an inviscid, isentropic fluid generated by a solid body whose surface executes prescribed vibrations is formulated and solved as a multiple scales perturbation problem, using the Mach number M based on the maximum surface velocity as the perturbation parameter. Following the idea of multiple scales, new "slow" spacial scales are introduced, which are defined as the usual physical spacial scale multiplied by powers of M. The governing nonlinear differential equations lead to a sequence of linear problems for the perturbation coefficient functions. However, it is shown that the higher order perturbation functions obtained in this manner will dominate the lower order solutions unless their dependence on the flow spacial scales is chosen in a certain manner. In particular, it is shown that the perturbation functions must satisfy an equation similar to Burgers' equation, with a slow spacial scale playing the role of the time-like variable. The method is illustrated by a simple one-dimensional example, as well as by three different cases of a vibrating sphere. The results are compared with solutions obtained by purely numerical methods and some insights provided by the perturbation approach are discussed.

Abgrall, R., On essentially non-oscillatory schemes on unstructured meshes: Analysis and implementation. ICASE Report No. 92-74, December 24, 1992, 37 pages. Submitted to the Journal of Computational Physics.

A few years ago, the class of Essentially Non-Oscillatory Schemes for the numerical simulation of hyperbolic equations and systems was constructed. Since then, some extensions have been made to multidimensional simulations of compressible flows, mainly in the context of very regular structured meshes. In this paper, we first recall and improve the results of an earlier paper about non-oscillatory reconstruction on unstructured meshes, emphasising the effective calculation of the reconstruction. Then we describe a class of numerical schemes on unstructured meshes and give some applications for its third order version. This demonstrates that a higher order of accuracy is indeed obtained, even on very irregular meshes.

Zhou, Ye, and George Vahala: Renormalization group estimates of transport coefficients in the advection of a passive scalar by incompressible turbulence. ICASE Report No. 93-1, February 22, 1993, 29 pages. Submitted to Physics of Fluids A.

The advection of a passive scalar by incompressible turbulence is considered using recursive renormalization group procedures in the differential subgrid shell thickness limit. It is shown explicitly that the higher order nonlinearities induced by the recursive renormalization group procedure preserve Galilean invariance. Differential equations, valid for the entire resolvable wavenumber k range, are determined for the eddy viscosity and eddy diffusivity coefficients and it is shown that higher order nonlinearities do not contribute as  $k \to 0$ , but have an essential role as  $k \to k_c$ , the cutoff wavenumber separating the resolvable scales from the subgrid scales. The recursive renormalization transport coefficients and the associated eddy Prandtl number are in good agreement with the k-dependent transport coefficients derived from closure theories and experiments.

Hall, Philip: On the initial stages of vortex wave interactions in highly curved boundary layer flows. ICASE Report No. 93-2, February 8, 1993, 31 pages. Submitted to Mathematika.

The nonlinear interaction equations describing vortex-Rayleigh wave interactions in highly curved boundary layers are derived. These equations describe a strongly nonlinear interaction between an inviscid wave system and a streamwise vortex. The coupling between the two structures is quite different than that found by Hall and Smith (1991) in the absence of wall curvature. Here the vortex is forced over a finite region of the flow rather than in the critical layer associated with the wave system. When the interaction takes place the wave system remains locally neutral as it moves downstream and it's self interaction drives a vortex field of the same magnitude as that driven by the wall curvature. This modification of the mean state then alters the wave properties and forces the wave amplitude to adjust itself in order that the wave frequency is constant. Solutions of the interaction equations are found for the initial stages of the interaction in the case when the wave amplitude is initially small. Our analysis suggests that finite amplitude disturbances can only exist when the vortex field is finite at the initial position where the interaction is stimulated.

Hall, Philip: On the instability of the flow in an oscillating tank of fluid. ICASE Report No. 93-3, February 8, 1993, 31 pages. Submitted to Journal of Fluid Mechanics.

The instability of a viscous fluid inside a rectangular tank oscillating about an axis parallel to the largest face of the tank is investigated in the linear regime. The flow is shown to be unstable to both longitudinal roll and standing wave instabilities. The particular cases of low and high oscillation frequencies are discussed in detail and the results obtained for the standing wave instability at low frequencies shed light on the corresponding steady flow instability problem. The relationship between the roll instability and convective or centrifugal instabilities in unsteady boundary layers is discussed. The eigenvalue problems associated with the roll and standing wave instabilities are solved using Floquet theory and a combination of numerical and asymptotic methods. The results obtained are compared to the recent experimental investigation of Bolton and Maurer (1992) which indeed provided the stimulus for the present investigation.

Jackson, T.L., Michéle G. Macaraeg, and M.Y. Hussaini: Role of acoustics in flame/vortex interactions. ICASE Report No. 93-4, February 10, 1993, 35 pages. Submitted to Journal of Fluid Mechanics.

The role of acoustics in flame/vortex interactions is examined via asymptotic analysis and numerical simulation. The model consists of a one-step, irreversible Arrhenius reaction between initially unmixed species occupying adjacent half-planes which are allowed to mix and react by convection and diffusion in the presence of an acoustic field or a time-varying pressure field of small amplitude. The main emphasis is on the influence of the acoustics on the ignition time and flame structure as a function of vortex Reynolds number and initial temperature differences of the reactants.

Nicol, David M., and Weizhen Mao: Isomorphic routing on a toroidal mesh. ICASE Report No. 93-5, February 10, 1993, 24 pages. Submitted to ORSA Journal on Computing.

We study a routing problem that arises on SIMD parallel architectures whose communication network forms a toroidal mesh. We assume there exists a set of k message descriptors  $\{(x_i, y_i)\}$ , where  $(x_i, y_i)$  indicates that the  $i^{th}$  message's recipient is offset from its sender by  $x_i$  hops in one mesh dimension, and  $y_i$  hops in the other. Every processor has k messages to send, and all processors use the same set of message routing descriptors. The SIMD constraint implies that at any routing step, every processor is actively routing messages with the same descriptors as any other processor. We call this *Isomorphic Routing*. Our objective is to find the isomorphic routing schedule with least makespan. We consider a number of variations on the problem, yielding complexity results from O(k) to NP-complete. Most of our results follow after we transform the problem into a scheduling problem, where it is related to other well-known scheduling problems.

Sun, Xian-He: Applications and accuracy of the parallel diagonal dominant algorithm. <u>ICASE</u> Report No. 93-6, February 25, 1993, 27 pages. Submitted to the International Conference on Parallel Processing.

The Parallel Diagonal Dominant (PDD) algorithm is a highly efficient, ideally scalable tridiagonal solver. In this paper, a detailed study of the PDD algorithm is given. First the PDD algorithm is introduced. Then the algorithm is extended to solve periodic tridiagonal systems. A variant, the reduced PDD algorithm, is also proposed. Accuracy analysis is provided for a class of tridiagonal systems, the symmetric and anti-symmetric Toeplitz tridiagonal systems. Implementation results show that the analysis gives a good bound on the relative error, and the algorithm is a good candidate for the emerging massively parallel machines.

Coward, Aidrian, and Philip Hall: On the nonlinear interfacial instability of rotating coreannular flow. ICASE Report No. 93-7, February 25, 1993, 39 pages. Submitted to Theoretical and Computational Fluid Dynamics.

The interfacial stability of rotating core-annular flows is investigated. The linear and nonlinear effects are considered for the case when the annular region is very thin. Both asymptotic and numerical methods are used to solve the flow in the core and film regions which are coupled by a difference in viscosity and density. The long-time behaviour of the fluid-fluid interface is determined by deriving its nonlinear evolution in the form of a modified Kuramoto-Sivashinsky equation. We obtain a generalization of this equation to three dimensions. The flows considered are applicable to a wide array of physical problems where liquid films are used to lubricate higher or lower viscosity core fluids, for which a concentric arrangement is desired. Linearized solutions show that the effects of density and viscosity stratification are crucial to the stability of the interface. Rotation generally destabilizes non-axisymmetric disturbances to the interface, whereas the centripetal forces tend to stabilize flows in which the film contains the heavier fluid. Nonlinear affects allow finite amplitude helically travelling waves to exist when the fluids have different viscosities.

Hu, Fang Q.: A numerical study of wave propagation in a confined mixing layer by Eigenfunction expansions. ICASE Report No. 93-8, March 5, 1993, 19 pages. Submitted to Physics of Fluids A.

It is well known that the growth rate of instability waves of a two-dimensional free shear layer is reduced greatly at supersonic convective Mach numbers. In previous works, it has been shown that new wave modes exist when the shear layers are bounded by a channel due to the coupling effect between the acoustic wave modes and the motion of the mixing layer. The present work studies the simultaneous propagation of multiple stability waves using numerical simulation. It is shown here that the co-existence of two wave modes in the flow field can lead to an oscillatory growth of disturbance energy with each individual wave mode propagating linearly. This is particularly important when the growth rates of the unstable waves are small. It is also shown here that the propagation of two neutrally stable wave modes can lead to a stationary periodic structure of r.m.s. fluctuations. In the numerical simulations presented here the forced wave modes are propagating at same frequency but with different phase velocities. In order to track the growth of each wave mode

as it propagates downstream, a numerical method which can effectively detect and separate the contribution of individual wave is given. It is demonstrated that by a least square fitting of the disturbance field with eigenfunctions the amplitude of each wave mode can be found. Satisfactory results as compared to linear theory are obtained.

Carpenter, Mark H., David Gottlieb, and Saul Abarbanel: Time-stable boundary conditions for finite-difference schemes solving hyperbolic systems: Methodology and application to high-order compact schemes. ICASE Report No. 93-9, March 5, 1993, 36 pages. Submitted to Journal of Computational Physics.

We present a systematic method for constructing boundary conditions (numerical and physical) of the required accuracy, for compact (Pade-like) high-order finite-difference schemes for hyperbolic systems. First a proper summation-by-parts formula is found for the approximate derivative. A "simultaneous approximation term" (SAT) is then introduced to treat the boundary conditions. This procedure leads to time-stable schemes even in the system case. An explicit construction of the fourth-order compact case is given. Numerical studies are presented to verify the efficacy of the approach.

Banks, H.T., and R.C. Smith: Well-posedness of a model for structural acoustic coupling in a cavity enclosed by a thin cylindrical shell. ICASE Report No. 93-10, March 9, 1993, 22 pages. Submitted to Journal of Mathematical Analysis and Applications.

A fully coupled mathematical model describing the interactions between a vibrating thin cylindrical shell and an enclosed acoustic field is presented. Because the model will ultimately be used in control applications involving piezoceramic actuators, the loads and material contributions resulting from piezoceramic patches bonded to the shell are included in the discussion. Theoretical and computational issues lead to the consideration of a weak form of the modeling set of partial differential equations (PDE's) and through the use of a semigroup formulation, well-posedness results for the system are obtained.

Burns, John A., and Yuh-Roung Ou: Effect of rotation rate on the forces of a rotating cylinder: Simulation and control. ICASE Report No. 93-11, March 19, 1993, 48 pages. Submitted to Physics of Fluids A.

In this paper we present numerical solutions to several optimal control problems for an unsteady viscous flow. The main thrust of this work is devoted to simulation and control of an unsteady flow generated by a circular cylinder undergoing rotary motion. By treating the rotate rate as a control variable we formulate two optimal control problems and use a central difference/pseudospectral transform method to numerically compute the optimal control rates. Several types of rotations are considered as potential controls and we show that a proper synchronization of forcing frequency with the natural vortex shedding frequency can greatly influence the flow. The results here indicate that using moving boundary controls for such systems may provide a feasible mechanism for flow control.

Leutenegger, Scott T., and Daniel Dias: A modeling study of the TPC-C benchmark. ICASE Report No. 93-12, March 24, 1993, 40 pages. To appear in SIGMOD '93 conference proceedings.

The TPC-C benchmark is a new benchmark approved by the TPC council intended for comparing database platforms running a medium complexity transaction processing workload. Some key aspects in which this new benchmark differs from the TPC-A benchmark are in having several transaction types, some of which are more complex than that in TPC-A, and in having data access skew. In this paper we present results from a modelling study of the TPC-C benchmark for both single node and distributed database management systems. We simulate the TPC-C workload to determine expected buffer miss rates assuming an LRU buffer management policy. These miss rates are then used as inputs to a throughput model. From these models we show the following: (i) We quantify the data access skew as specified in the benchmark and show what fraction of the accesses go to what fraction of the data. (ii) We quantify the resulting buffer hit ratios for each relation as a function of buffer size. (iii) We show that close to linear scale-up (about 3% from the ideal) can be achieved in a distributed system, assuming replication of a read-only table. (iv) We examine the effect of packing hot tuples into pages and show that significant price/performance benefit can be thus achieved. (v) Finally, by coupling the buffer simulations with the throughput model, we examine typical disk/memory configurations that maximize the overall price/performance.

Borggaard, Jeff, John A. Burns, Eugene Cliff, and Max Gunzburger: Sensitivity calculations for a 2D, inviscid, supersonic forebody problem. ICASE Report No. 93-13, March 23, 1993, 13 pages. To appear in the Proceedings of the AMS-IMS-SIAM Summer Conference on Distributed Parameter Control, SIAM, 1993.

In this paper, we discuss the use of a sensitivity equation method to compute derivatives for optimization based design algorithms. The problem of designing an optimal forebody simulator is used to motivate the algorithm and to illustrate the basic ideas. Finally, we indicate how an existing CFD code can be modified to compute sensitivities and a numerical example is presented.

Nicol, David M., and Daniel L. Palumbo: Reliability analysis of complex models using SURE bounds. ICASE Report No. 93-14, March 23, 1993, 27 pages. Submitted to IEEE Transactions on Reliability.

As computer and communications systems become more complex it becomes increasingly more difficult to analyze their hardware reliability, because simple models may fail to adequately capture subtle but important model features. This paper describes a number of ways we have addressed this problem for analyses based upon White's SURE theorem. We point out how reliability analysis based on SURE mathematics can be extracted from a general C language description of the model behavior, how it can attack very large problems by accepting recomputation in order to reduce memory usage, how such analysis can be parallelized both on multiprocessors and on networks of ordinary workstations, and observe excellent performance gains by doing so. We also discuss how the SURE theorem supports efficient Monte Carlo based estimation of reliability, and show the advantages of the method.

# ICASE COLLOQUIA

October 1, 1992 - March 31, 1993

Name/Affiliation/Title	Date
Bernard Traversat, Superconducting Super Collider Laboratory "Parallel Computing Experience on a Heterogeneous Computing Farm"	October 5
Nick Trefethen, Cornell University "Linear but Non-Modal Effects in Hydrodynamic Stability"	October 5
Lois Curfman, Institute for Parallel Computation, University of Virginia "Solution of Convective-Diffusive Flow Problems with Newton-Like Methods"	October 9
Swami Nigam, Indian Institute of Technology, Madras "Circulation, Vorticity and Helicity"	October 19
Swami Nigam, Indian Institute of Technology, Madras "Sphere Theorems for Stokes Flows"	October 20
Gerard Degrez, von Karman Institute for Fluid Dynamics, Belgium "Experimental and Numerical Research on Supersonic/Hypersonic Flows at the Von Karman Institute for Fluid Dynamics"	October 21
Forman Williams, University of California, San Diego "Hydrogen Diffusion-Flame Studies for High-Speed Propulsion"	October 22
Hsin-Chu Chen, University of Southwestern Louisiana "Parallel Matrix/Domain Decomposition Methods for Finite Element Computation"	October 26
G. S. Triantafyllou, The Benjamin Levich Institute, The City College of New York "Non-Linear Dynamics of Shear Flow with a Free Surface"	October 30
John Burns, Virginia Polytechnic Institute & State University "Computational Issues in Optimization Based Control and Design of Partial Differential Equations"	November 4
Charles Weatherford, Florida A & M University "Partial Differential Equation Approach to Electron-Molecule Scattering"	December 7

Name/Affiliation/Title	Date
Piyush Mehrotra, ICASE  "High Performance Fortran"	December 8
Richard Sincovec, Oak Ridge National Laboratory "Oak Ridge National Laboratory's Center for Computational Science"	December 10
Christopher Tam, Florida State University "Dispersion-Relation-Preserving Finite Difference Schemes for Computational Aeroacoustics"	December 11
S. Elghobashi, University of California, Irvine "On the Two-Way Interaction Between Homogeneous Turbulence and Dispersed Solid Particles"	December 14
S. Nagendra, Virginia Polytechnic Institute and State University "Discrete-Continuous Optimum Design of Stiffened Composite Panels by a Genetic Algorithm Approach"	December 16
Oleg S. Ryzhov, Rensselaer Polytechnic Institute "On the Landau-Goldstein Singularity and Marginal Separation"	January 11
Thomas Fahringer, University of Vienna "A Static Performance Estimator for Parallel Fortran Program"	January 13
Hudong Chen, Dartmouth College "Lattice Gas and Lattice Boltzman Automation Methods - A New Way for Studying Fluid Flows"	January 14
Ye Zhou, ICASE "Introduction to Renormalization Group Method in Turbulence"	January 15 and 22
Steven A. Orszag, Princeton University "Numerical Simulation of Electronic Chip Manufacturing Processes"	January 19
Gal Berkooz, Cornell University  "Applications of Wavelets to Dynamical Models and Simulations of Turbulence"	January 25
Manoucher Ghamsari, Christopher Newport University "Fractals, Chaos, and Complex Dynamics"	January 28
Jay C. Webb, Florida State University "Aspects of Direct Numerical Simulation of Supersonic Jet Flow"	January 29

Name/Affiliation/Title	Date
D. Glenn Lasseigne, Old Dominion University "Interaction of Disturbances with a Detonation or Shock Wave Attached to a Wedge"	February 3
Alex Solomonoff, University of Minnesota  "Reconstruction of a Discontinuous Function from a Few Fourier Coefficients using Bayesian Estimation"	February 8
Lawrence L. Green, NASA LaRC "Application of Automatic Differentiation to Advanced CFD Codes"	February 10
Matthew Haines, Colorado State University "On the Design on Distributed Memory Sisal"	February 12
Eran Gabber, Tel-Aviv University "A Portable and Efficient Programming Environment for Multiprocessors"	February 16
Mujeeb R. Malik, High Technology Corporation "Crossflow Disturbances in 3D Boundary Layers: Nonlinear Development, Wave-Interaction and Secondary Instability"	February 17
V. Venkatakrishnan, CSC/NASA Ames Research Center "On the Accuracy of Limiters and Convergence to Steady State Solutions"	February 25
Anthony T. Patera, Massachusetts Institute of Technology "Construction, Validation, and Application of Computer Simulation Surrogates"	March 1
Gianfranco Ciardo, The College of William and Mary "A Decomposition Approach for Stochastic Petri Net Models"	March 4
Daniel Quinlan, University of Colorado at Denver "Parallel Self Adaptive Mesh Refinement Using C++ Class Libraries for Abstraction of Parallelism and Self Adaptive Mesh Refinement"	March 4
Steven H. Frankel, SUNY at Buffalo "Probabilistic and Deterministic Description of Reacting Turbulence"	March 5
Sharath S. Girimaji, A.S.&M. Inc. "Towards Understanding Turbulent Scalar Mixing"	March 10
Bob Felderman, Information Sciences Institute, University of California "ATOMIC, A Low-Cost, Very-High-Speed LAN"	March 12

Name/Affiliation/Title	Date
Carlos E. Orozco, Carnegie-Mellon University "A Highly Parallel Reduced SQP Method for Aerodynamic Design"	March 12
Keh-ming Shyue, University of Washington "Front Tracking Based on High Resolution Wave Propagation Method"	March 15
Peter Eiseman, Program Development Corporation "Structured Grid Generation is Alive!"	March 19
G. Balakrishnan, University of California, San Diego "Studies of Laminar Hydrogen-Air Diffusion Flames"	March 22
F. Farassat, NASA Langley Research Center "Generalized Functions in Aerodynamics and Aeroacoustics"	March 24
Jerry Yan, NASA Ames Research Center "Performance Evaluation of Parallel Programs: The Ames InstruMentation System"	March 25
Nicholas J. Higham, University of Manchester "Open Problems in Parallel Numerical Linear Algebra"	March 26

#### OTHER ACTIVITIES

A workshop on Combustion, cosponsored by ICASE and NASA Langley Research Center was held October 12-14, 1992 at the OMNI Hotel in Newport News, Virginia. Sixty-one people attended this workshop.

The workshop theme was Modeling in High Speed Propulsion and the objective was to discuss the basic physical phenomena of flow fields associated with scramjets and/or oblique detonation wave engines (ODWE) as well as to discuss models thereof to study them in isolation.

A volume of the proceedings from this workshop will be published in the near future.

A Wavelet Short Course, cosponsored by ICASE and NASA Langley Research Center, was held February 22-26, 1993 at the Holiday Inn in Hampton, Virginia. There were 95 attendees. The objective of this course was to give scientists and engineers a practical understanding of wavelets, their origins, their purpose, their use, and their prospects.

A volume consisting of the course notes will be published in the near future.

#### **ICASE STAFF**

#### I. ADMINISTRATIVE

M. Yousuff Hussaini, Director. Ph.D., Mechanical Engineering, University of California, 1970.

Linda T. Johnson, Office and Financial Administrator

Etta M. Blair, Personnel/Accounting Supervisor

Cynthia C. Cokus, PC System Coordinator

Barbara A. Cardasis, Administrative Secretary

Tamiko J. Hackett, Contract Accounting Clerk

Rachel A. Lomas, Payroll and Accounting Clerk

Rosa H. Milby, Executive Secretary/Visitor Coordinator

Shelly D. Millen, Technical Publications Secretary

Emily N. Todd, Conference Manager

# II. SCIENCE COUNCIL for APPLIED MATHEMATICS and COMPUTER SCIENCE

Ashwani Kapila, Professor, Department of Mathematics and Science, Rensselaer Polytechnic Institute.

James P. Kendall, Jet Propulsion Laboratory.

Heinz-Otto Kreiss, Professor, Department of Mathematics, University of California at Los Angeles.

Sanjoy Mitter, Professor of Electrical Engineering, Massachusetts Institute of Technology.

Robert O'Malley, Jr., Chairman, Department of Applied Mathematics, University of Washington.

Stanley J. Osher, Professor, Mathematics Department, University of California.

Eli Reshotko, Department of Mechanical and Aerospace Engineering, Case Western University.

John Rice, Head, Department of Computer Science, Purdue University.

Ahmed Sameh, Professor, Center for Supercomputing Research and Development, University of Illinois at Urbana.

M. Y. Hussaini, Director, Institute for Computer Applications in Science and Engineering, NASA Langley Research Center.

# III. ASSOCIATE MEMBERS

Saul S. Abarbanel, Professor, Department of Applied Mathematics, Tel-Aviv University, Israel.

H. Thomas Banks, Director, Center for Research in Scientific Computation, North Carolina State University.

David Gottlieb, Professor, Division of Applied Mathematics, Brown University.

Peter D. Lax, Professor, Courant Institute of Mathematical Sciences, New York University.

## V. SENIOR STAFF SCIENTIST

Gordon Erlebacher - Ph.D., Plasma Physics, Columbia University, 1983. Computational Fluid Dynamics. (November 1989 to November 1994)

Dimitri Mavriplis - Ph.D., Mechanical and Aerospace Engineering, Princeton University, 1988. Grid Techniques for Computational Fluid Dynamics. (February 1987 to September 1995)

Piyush Mehrotra - Ph.D., Computer Science, University of Virginia, 1982. Programming Languages for Multiprocessor Systems. (January 1991 to September 1994)

Charles G. Speziale - Ph.D., Aerospace and Mechanical Sciences, Princeton University, 1978. Fluid Dynamics with Emphasis on Turbulence Modeling and the Transition Process. (September 1987 to November 1992)

Shlomo Ta'asan - Ph.D., Applied Mathematics, The Weizmann Institute of Science, 1985. Multigrid Methods for Partial Differential Equations. (July 1991 to July 1994)

John R. Van Rosendale - Ph.D., Computer Science, University of Illinois, 1980. Parallel Systems and Algorithms. (July 1989 to September 1993)

#### VI. SCIENTIFIC STAFF

Fabio Bertolotti - Ph.D., Mechanical Engineering, Ohio State University, 1991. Stability Theory in Fluid Mechanics, (September 1991 to September 1993)

Kurt M. Bryan - Ph.D., Mathematics, University of Washington, 1990. Theoretical and Computational Methods for Inverse Problems. (August 1990 to August 1993)

Leon M. Clancy - B.S., Mechanical Engineering, University of Washington, 1971. System Manager. (December 1989 to Present)

Michael S. Cokus - M.S., Computer Science, College of William and Mary, 1990. Applied Computer Science, in particular, System Software. (November 1992 to November 1994)

Thomas W. Crockett - B.S., Mathematics, College of William and Mary, 1977. Parallel Systems Research. (February 1987 to September 1993)

Subhendu Das - M.S., Computer Science, College of William and Mary, 1990. Parallel Tools and Environments for Unstructured Scientific Computations. (June 1991 to October 1992)

Phillip M. Dickens - Ph.D., Computer Science, University of Virginia, 1992. System Software. (January 1993 to January 1995)

Ulf R. Hanebutte - Ph.D., Mechanical Engineering, Northwestern University, 1992. Parallel Numerical Algorithms. (October 1992 to October 1994)

Scott T. Leutenegger - Ph.D., Computer Science, University of Wisconsin-Madison, 1990. Performance Analysis. (September 1992 to September 1994)

Stephen R. Otto - Ph.D., Mathematics, Exeter University, England, 1991. Asymptotic Theories of Stability and Transition. (November 1991 to November 1993)

James Quirk - Ph.D., Computational Fluid Dynamics, Cranfield Institute of Technology, 1991. Adaptive Methods for Partial Differential Equations. (June 1991 to September 1994)

Mathew Rosing - Ph.D., Computer Science, University of Colorado, Boulder, 1991. Tools and Compilers for Scalable Multiprocessors. (November 1991 to June 1994)

J. Ray Ristorcelli - Ph.D., Mechanical and Aerospace Engineering, Cornell University, 1991. Fluid Mechanics. (December 1992 to December 1994)

Sutanu Sarkar - Ph.D., Mechanical and Aerospace Engineering, Cornell University, 1988. Fluid Dynamics, Turbulence Modeling, Compressible Turbulence. (September 1988 to December 1992)

Ralph C. Smith - Ph.D., Mathematics, Montana State University, 1990. Theoretical and Computational Issues Associated with Feedback Control Problems. (August 1990 to August 1993)

Xian-He Sun - Ph.D., Computer Science, Michigan State University, 1990. Applied Computer Science. (September 1992 to September 1994)

Alan Sussman - Ph.D., Computer Science, Carnegie-Mellon University, 1991. Quantifying and Predicting Performance of Realistic Applications on Distributed Memory Parallel Computers. (August 1991 to December 1992)

Ye Zhou - Ph.D., Physics, College of William and Mary, 1987. Fluid Mechanics. (October 1992 to October 1994)

#### VII. VISITING SCIENTISTS

Shapour Azarm - Ph.D., Mechanical Engineering, University of Michigan, 1977. Associate Professor, Department of Mechanical Engineering, University of Maryland. Optimization-Based Design. (August to December 1992)

Stanley A. Berger - Ph.D., Applied Mathematics, Brown University, 1959. Professor, Department of Mechanical Engineering, University of California-Berkeley. Analytical & Numerical Studies of Vortex Breakdown. (October 1992 to January 1993)

Barbara Chapman - M.S., Mathematics, University of Canterbury, Christchurch, New Zealand, 1985. Research Associate, Computer Science Department, University of Vienna. Compiler Development for Multiprocessors. (February to March 1993)

Peter W. Duck - Ph.D., Fluid Mechanics, University of Southampton, United Kingdom, 1975. Lecturer in Mathematics, Department of Mathematics, University of Manchester, United Kingdom. Numerical Solution of Unsteady Boundary Layer Equations. (November to December 1992)

Paul Hammerton - Ph.D., Applied Mathematics, University of Cambridge, United Kingdom, 1990. Research Associate, Department of Applied Mathematics and Theoretical Physics, University of Cambridge, United Kingdom. Propagation of Sonic Booms Through a Real Atmosphere. (February to March 1993)

Thomas L. Jackson - Ph.D., Mathematics, Rensselaer Polytechnic Institute, 1985. Associate Professor, Department of Mathematics and Statistics, Old Dominion University. Fluid Mechanics. (December 1992 to January 1994)

Geoffrey M. Lilley - Ph.D., Engineering, Imperial College, London, England, 1945. Professor Emeritus, Department of Aeronautics and Astronautics of Southampton, United Kingdom. Fluid Mechanics. (August to December 1992)

Eric O. Morano - Ph.D., Engineering, University of Nice, France, 1992. Ph.D. INRIA Fellowship. INRIA, France. Computational Aerodynamics. (February 1993 to Present)

John V. Shebalin - Ph.D., Physics, College of William & Mary, 1982. Aerospace Technologist, NASA Langley Research Center. Compressible Turbulence. (July 1992 to Present)

Nicolas G. Verhaagen - Ph.D., Aeronautics, Delft University of Technology, The Netherlands, 1970. Research Scientist, Department of Aerospace Engineering, Delft University of Technology, The Netherlands. Experimental and Numerical Studies of Vortex Flows. (August to October 1992)

Hong Zhang-Sun - Ph.D., Applied Mathematics, Michigan State University, 1989. Assistant Professor, Department of Mathematical Sciences, Clemson University. Parallel Numerical Algorithms. (September 1992 to Present)

## VIII. CONSULTANTS

Alvin Bayliss - Ph.D., Mathematics, New York University, 1975. Associate Professor, Technological Institute, Northwestern University. Fluid Mechanics [Numerical Methods for Partial Differential Equations]

John D. Buckmaster - Ph.D., Applied Mathematics, Cornell University, 1969. Professor, Department of Aeronautical and Astronautical Engineering, University of Illinois. Fluid Mechanics [Mathematical Combustion]

John A. Burns - Ph.D., Mathematics, University of Oklahoma, 1973. Professor, Virginia Polytechnic Institute and State University. Applied & Numerical Mathematics [Numerical Methods in Feedback Control and Parameter Estimation]

Thomas C. Corke - Ph.D., Mechanical and Aerospace Engineering, Illinois Institute of Technology, 1981. Professor, Department of Mechanical and Aerospace Engineering, Armour College of Engineering, Illinois Institute of Technology. Fluid Mechanics [Transition and Stability to Turbulence]

William O. Criminale - Ph.D., Aeronautics, The John Hopkins University, 1960. Professor, Department of Applied Mathematics, University of Washington. Fluid Mechanics [Stability and Transition]

Ayodeji O. Demuren - Ph.D., Mechanical Engineering, Imperial College London, United Kingdom, 1979. Associate Professor, Department of Mechanical Engineering and Mechanics, Old Dominion University. Fluid Mechanics [Numerical Modeling of Turbulent Flows]

Peter R. Eiseman - Ph.D., Mathematics, University of Illinois, 1970. Senior Research Scientist and Adjunct Professor, Department of Applied Physics and of Nuclear Engineering, Columbia University. Applied & Numerical Mathematics [Computational Fluid Dynamics]

James F. Geer - Ph.D., Applied Mathematics, New York University, 1967. Professor, Systems Science and Mathematical Sciences, Watson School of Engineering, Applied Science and Technology, SUNY-Binghamton. Fluid Mechanics [Perturbation Methods and Asymptotic Expansions of Solutions to Partial Differential Equations]

Chester E. Grosch - Ph.D., Physics - Fluid Dynamics, Stevens Institute of Technology, 1967. Professor, Department of Computer Science and Slover Professor, Department of Oceanography, Old Dominion University. Fluid Mechanics [Computational Fluid Mechanics and Algorithms for Array Processor Computers]

Philip Hall - Ph.D., Mathematics, Imperial College, England, 1973. Professor, Department of Mathematics, University of Manchester, England. Fluid Mechanics [Computational Fluid Dynamics]

Amiram Harten - Ph.D., Mathematics, New York University, 1974. Associate Professor, Department of Mathematics, Tel-Aviv University, Israel. Applied & Numerical Mathematics [Numerical Solution for Partial Differential Equations]

Fang Q. Hu - Ph.D., Applied Mathematics, Florida State University, 1990. Assistant Professor, Department of Mathematics and Statistics, Old Dominion University. Fluid Mechanics [Instability and Transition]

Harry F. Jordan - Ph.D., Physics, University of Illinois, 1967. Professor Department of Electrical and Computer Engineering, University of Colorado at Boulder. Computer Science [Parallel Computation]

Daniel D. Joseph - Ph.D., Mechanical Engineering, Illinois Institute of Technology, 1993. Russell J. Penrose Professor of Aerospace Engineering and Mechanics, Department of Aerospace Engineering and Mechanics, University of Minnesota. Fluid Mechanics.

Ashwani K. Kapila - Ph.D., Theoretical and Applied Mechanics, Cornell University, 1975. Associate Professor, Department of Mathematical Sciences, Rensselaer Polytechnic Institute. Fluid Mechanics [Ordinary and Partial Differential Equations, Asymptotic Methods]

Ken Kennedy - Ph.D., Computer Science, New York University, 1971. Chairman, Department of Computer Science, Rice University. Computer Science [Parallel Compilers and Languages]

Edward J. Kerschen - Ph.D., Mechanical Engineering, Stanford University, 1978. Associate Professor, Department of Aerospace and Mechanical Engineering, University of Arizona. Flow Dynamics.

David E. Keyes - Ph.D., Applied Mathematics, Harvard University, 1984. Assistant Professor, Mechanical Engineering, Yale University. Computer Science [Parallelization of Numerical Procedures Appropriate for the Study of Combustion]

Heinz-Otto Kreiss - Ph.D., Mathematics, Royal Institute of Technology, Sweden 1960. Professor, Department of Applied Mathematics, California Institute of Technology. Applied & Numerical Mathematics [Numerical Analysis]

David G. Lasseigne - Ph.D., Applied Mathematics, Northwestern University, 1985. Assistant Professor, Department of Mathematics and Statistics, Old Dominion University. Fluid Mechanics [Computational Fluid Dynamics]

Anthony Leonard - Ph.D., Nuclear Engineering, Stanford University, 1963. Professor of Aeronautics, California Institute of Technology. Fluid Mechanics [Fluid Physics]

Robert W. MacCormack - M.S., Mathematics, Stanford University. Professor, Department of Aeronautics and Astronautics, Stanford University. Fluid Mechanics [Computational Fluid Dynamics and Numerical Analysis]

Catherine A. Mavriplis - Ph.D., Aeronautics and Astronautics, Massachusetts Institute of Technology, 1989. Assistant Professor, Department of Civil, Mechanical and Environmental Engineering, The George Washington University. Fluid Mechanics [Computational Fluid Dynamics]

Mark V. Morkovin - Ph.D., Applied Mathematics, University of Wisconsin, 1942. Professor Emeritus, Department of Mechanical and Aerospace Engineering, Illinois Institute of Technology. Transition Process in Aerodynamics.

David M. Nicol - Ph.D., Computer Science, University of Virginia, 1985. Professor, Department of Computer Science, College of William and Mary. Computer Science [Mapping Algorithms onto Parallel Computing Systems]

James M. Ortega - Ph.D., Mathematics, Stanford University, 1962. Professor and Chairman, Department of Applied Mathematics, University of Virginia. Computer Science [Numerical Analysis of Methods for Parallel Computers]

Stanley J. Osher - Ph.D., Functional Analysis, New York University, 1966. Professor, Department of Mathematics, University of California at Los Angeles. Applied & Numerical Mathematics [Methods for the Numerical Analysis of Partial Differential Equations]

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Demetrius Papageorgiou - Ph.D., Mathematics, University of London, 1985. Assistant Professor, Department of Mathematics, New Jersey Institute of Technology. Fluid Mechanics [Computational Fluid Dynamics]

Ugo Piomelli - Ph.D., Mechanical Engineering, Stanford University 1987. Professor, Department of Mechanical Engineering, University of Maryland. Fluid Mechanics [Subgrid Scale Reynold's Stress Modelling and Large Eddy Simulation of Turbulent Flows]

Daniel A. Reed - Ph.D., Computer Science, Purdue University, 1983. Assistant Professor, Department of Computer Science, University of Illinois. Computer Science [Parallel Processing]

Helen L. Reed - Ph.D., Engineering Mechanics, Virginia Polytechnic Institute and State University, 1981. Associate Professor, Department of Mechanical Engineering, Arizona State University. Fluid Mechanics [Computational Fluid Dynamics]

Eli Reshotko - Ph.D., Aeronautics and Physics, California Institute of Technology, 1960. Kent H. Smith Professor of Engineering, Case Western Reserve University. Fluid Mechanics [High Speed Aerodynamics with an Emphasis on Transition, Turbulence and Combustion]

Philip L. Roe - Ph.D., Aeronautics, University of Cambridge, United Kingdom, 1962. Professor, Department of Aerospace Engineering, University of Michigan. Fluid Mechanics [Numerical Analysis and Algorithms]

Joel E. Saltz - Ph.D., Computer Science, Duke University, 1985. Professor, Department of Computer Science, University of Maryland. Computer Science [System Software]

Sutanu Sarkar - Ph.D., Mechanical and Aerospace Engineering, Cornell University, 1988. Professor, Department of AMES, University of California, San Diego. Fluid Mechanics [Turbulence in High-Speed Compressible Fluid Dynamics]

Robert B. Schnabel - Ph.D., Computer Science, Cornell University, 1977. Chair, Computer Science Department, University of Colorado-Boulder. Computer Science [Numerical Methods for Optimization]

Jeffrey S. Scroggs - Ph.D., Computer Science, University of Illinois at Urbana, 1988. Assistant Professor, Department of Mathematics, North Carolina State University. Computer Science [Domain Decomposition Techniques for Partial Differential Equations]

Joseph E. Shepherd - Ph.D., Applied Physics, California Institute of Technology, 1980. Associate Professor, Department of Mechanical Engineering, Rensselaer Polytechnic Institute. Fluid Mechanics [Combustion]

Chi-Wang Shu - Ph.D., Mathematics, University of California, Los Angeles, 1986. Associate Professor, Division of Applied Mathematics, Brown University. Applied & Numerical Mathematics [Numerical Partial Differential Equations and Computational Fluid Dynamics]

Katepalli R. Sreenivason - Ph.D., Aeronautical Engineering, Indian Institute of Science, 1975. Professor and Chairman, Department of Mechanical Engineering, Yale University. Fluid Mechanics [Transition and Turbulence]

Alan L. Sussman - Ph.D., Computer Science, Carnegie Mellon University, 1991. Assistant Professor, Department of Computer Science, University of Maryland. Computer Science [Parallel Computing]

Saleh Tanveer - Ph.D., Applied Mathematics, California Institute of Technology, 1984. Professor, Department of Mathematics, Ohio State University. Fluid Mechanics [Problems for Crystal Growth]

Lu Ting - Ph.D., Aeronautics, New York University, 1951. Professor, Courant Institute of Mathematical Sciences, New York University. Fluid Mechanics.

Lloyd N. Trefethen - Ph.D., Computer Science, Stanford University, 1982. Professor, Department of Computer Science, Cornell University. Fluid Mechanics [Numerical Methods for Partial Differential Equations]

Eli Turkel - Ph.D., Applied Mathematics, New York University, 1970. Associate Professor, Department of Applied Mathematics, Tel-Aviv University, Israel. Applied & Numerical Mathematics [Computational Fluid Dynamics]

George M. Vahala - Ph.D., Physics, University of Iowa, 1972. Professor, Department of Physics, The College of William & Mary. Fluid Mechanics [Group Renormalization Methods for Turbulence Approximation]

Bram van Leer - Ph.D., Theoretical Astrophysic, Leiden State University, The Netherlands, 1970. Professor, Department of Aerospace Engineering, University of Michigan. Applied & Numerical Mathematics [Computational Fluid Dynamics]

Forman A. Williams - Ph.D., Engineering Sciences, California Institute of Technology, 1958. Professor, Department of Applied Mechanics and Engineering Sciences and Director, Center for Energy and Combustion Research, University of California, San Diego. Fluid Mechanics [Combustion]

Hans Zima - Ph.D., Mathematics, University of Vienna, Austria, 1964. Professor, Computer Science Department, University of Vienna, Austria. Computer Science [Compiler Development for Parallel and Distributed Multiprocessors]

Mohammad Zubair - Ph.D., Computer Science, Indian Institute of Technology, New Delhi, India, 1987. Assistant Professor, Department of Computer Science, Old Dominion University. Computer Science [Performance of Unstructured Flow-Solvers on Multi Processor Machines]

# IX. STUDENT ASSISTANTS

Avik Banerjee - Graduate Student at Hampton University. (May 1992 to Present)

John Otten - Graduate Student at The College of William and Mary. (May 1991 to January 1993)

#### X. GRADUATE STUDENTS

Eyal Arian - Graduate Student at Weizmann Institute of Science. Israel. (March 1993 to Present)

Thomas M. Brown - Graduate Student at Vanderbilt University. (October 1992 to Present)

Zigo Haras - Graduate Student at Weizmann Institute of Science. Israel. (December 1992)

Angelo Iollo - Graduate Student at Politecnico di Torino. (January 1993 to Present)

Frank P. Kozusko - Graduate Student at Old Dominion University. (October 1992 to Present)

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